WORLD INTELLECTUAL PROPERTY ORGANIZATION International Bureau



	HED I	
(51) International Patent Classification 7:	١	(11) International Publication Number: WO 00/26246
C07K 14/00	A2	(43) International Publication Date: 11 May 2000 (11.05.00
(21) International Application Number: PCT/US (22) International Filing Date: 5 November 1999 (LLP, 28 State Street, Boston, MA 02109 (US).
(30) Priority Data: 60/107,219 5 November 1998 (05.11.98 (63) Related by Continuation (CON) or Continuation-in (CIP) to Earlier Application US 60/107,2 Filed on 5 November 1998 ((71) Applicants (for all designated States except US): CORPORATION [US/US]; 1613 Prospect Parky Collins, CO 80525 (US). NORTHWESTERN US/US/US/US/US/US/US/US/US/US/US/US/US/U	HESK way, Founive 201 (U) Theodo IL 606 O Oakt an-Pici	(81) Designated States: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU; CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG). Published Without international search report and to be republished upon receipt of that report.

(54) Title: THREE-DIMENSIONAL MODEL OF A FC EPSILON RECEPTOR ALPHA CHAIN AND USES THEREOF

(57) Abstract

The present invention includes three-dimensional models of antibody receptor proteins, such as FccRIa proteins, and methods to produce such models. The present invention also includes muteins having increased stability and/or antibody binding activity, as well as methods to produce such muteins, preferably using information derived from three-dimensional models of the present invention. Also included are nucleic acid sequences encoding muteins of the present invention and use of those sequences to produce such muteins. Also included is the use of the model to identify compounds that inhibit the binding of an antibody receptor protein to an antibody. The present invention also includes uses of such muteins and inhibitory compounds, for example, in methods to diagnose and protect animals from allergy and other abnormal immune responses.

BEST AVAILABLE COPY

FOR THE PURPOSES OF INFORMATION ONLY

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the

AL AM AT AU AZ BA BB BE BF BG BJ BR CA CF CG CH CI CM CN CU CZ DE DK EE	Albania Amenia Austria Australia Azerbaijan Bosnia and Herzegovina Barbados Belgium Burkina Faso Bulgaria Benin Brazil Belarus Canada Central African Republic Congo Switzerland Côte d'Ivoire Cameroon China Cuba Czech Republic Germany Denmark Estonia	ES FI FR GA GB GE GH GN GR HU IS IT JP KE KG KP KR LC LI LK	Spain Finland France Gabon United Kingdom Georgia Ghana Guinea Greece Hungary Ireland Israel Iceland Italy Japan Kenya Kyrgyzstan Democratic People's Republic of Korea Republic of Korea Kazakstan Saint Lucia Liechtenstein Sri Lanka Liberia	LS LT LU LV MC MD MG MK ML MN MR MW MX NE NL NO NZ PL PT RO RU SD SE SG	Lesotho Lithuania Luxembourg Larvia Monaco Republic of Moldova Madagascar The former Yugoslav Republic of Macedonia Mali Mongolia Mauritania Malawi Mexico Niger Netherlands Norway New Zealand Poland Portugal Romania Russian Federation Sudan Sweden Singapore	SI SK SN SZ TD TG TJ TM TR TT UA UG US UZ VN YU ZW	Slovenia Slovakia Senegal Swaziland Chad Togo Tajikistan Turkey Trinidad and Tobago Ukraine Uganda United States of America Uzbekistan Viet Nam Yugoslavia Zimbabwe
-------------------------------------------------------------------------	-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------	-------------------------------------------------------------	-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------	-------------------------------------------------------------------------	-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------	----------------------------------------------------------------------------------------------------	---------------------------------------------------------------------------------------------------------------------------------------------------------------------

WO 00/26246 PCT/US99/26203

THREE-DIMENSIONAL MODEL OF A Fc EPSILON RECEPTOR ALPHA CHAIN AND USES THEREOF

This invention was made at least in part with government support under NIH Grant No. RO1 AI38972, awarded by the National Institutes of Health to Northwestern University. The government has certain rights to this invention.

-FIELD OF THE INVENTION

The present invention relates to a crystal and a three-dimensional (3-D) model of a Fc epsilon receptor alpha chain as well as to the use of that model to produce muteins and inhibitors useful in the diagnosis and treatment of allergy and the regulation of other immune responses in an animal.

BACKGROUND OF THE INVENTION

10

25

Antibody Fc-receptors (FcRs) play an important role in the immune response by coupling the specificity of secreted antibodies to a variety of cells of the immune system. A number of cell types, including macrophages, mast cells, eosinophils, and basophils, express membrane-bound FcRs at their surfaces. The binding of antibodies to FcRs provides antigen-specificity to these cells, which upon activation release further cell-specific mediators of the immune response, such as interleukins, initiators of inflammation, leukotrienes, prostaglandins, histamines, or cytotoxic proteins. The adoptive specificity of the FcRs allows a combinatorial approach to pathogen elimination, by coupling the diversity of antibody antigen-recognition sites to the variety of cell-types expressing these receptors.

FcR-initiated mechanisms are important in normal immunity to infectious disease as well as in allergies, antibody-mediated tumor recognition, autoimmune diseases, and other diseases in which immune responses are abnormal (i.e., not regulated). Recent experiments with transgenic mice have demonstrated that the FcRs control key steps in the immune response, including antibody-directed cellular cytotoxicity and inflammatory cascades associated with the formation of immune complexes; see, for example, Ravetch et al., 1998, *Annu Rev Immunolo 16*, 421-432. Receptors that bind IgG (FcgRI, FcgRII, and FcgRIII, known collectively as FcgRs) mediate a variety of inflammatory reactions, regulate B-cell activation, and also trigger hypersensitivity reactions. The high affinity Fc epsilon receptor (also known as the IgE

receptor or FceRI) is associated with the activation of mast cells and the triggering of allergic reactions and anaphylactic shock. Knockout mice for the FceRI alpha chain (FcεRIα) are unable to mount IgE-mediated anaphylaxis (see for example, Dombrowicz et al., 1993, Cell 75, 969-976), although FcgRs are still able to activate mast cells (see, for example, Dombrowicz et al., 1997, J. Clin. Invest. 99, 915-925; Oettgen et al., 1994, Nature 370, 367-370). FceRI has also been shown to trigger anti-parasitic reactions from platelets and eosinophils as well as deliver antigen into the MHC class II presentation pathway for the activation of T cells; see, for example, Gounni et al., 1994, Nature 367, 183-186; Joseph et al., 1997, Eur. J. Immunol. 27, 2212-2218; Maurer et al., 1998, J. Immunol. 161, 2731-2739. The b-subunit of FceRI has been associated with asthma in 10 genetic studies; see, for example, Hill et al., 1996, Hum. Mol. Genet. 5, 959-962; Hill et al., 1995, Bmj 311, 776-779; Kim et al., 1998, Curr. Opin. Pulm. Med. 4, 46-48; Mao et al., 1998, Clin. Genet. 53, 54-56; Shirakawa et al., 1994, Nat. Genet. 7, 125-129. A significant fraction of the population (~20%) may be affected by allergies, and this century has seen a substantial increase in asthma. Since IgE binding to FceRI is a requisite event in the reaction to different allergens, therapeutic strategies aimed at inhibiting FceRI could provide a useful treatment for these diseases. For example, monoclonal antibodies that target IgE and block receptor binding have shown therapeutic potential; see, for example, Heusser et al., 1997, Curr. Opin. Immunol. 9, 20 805-813.

FceRI is found as a tetrameric (abg₂) or trimeric (ag₂) membrane bound receptor on the surface of mast cells, basophils, eosinophils, langerhans cells and platelets. The alpha chain, also referred to as FceRIα, of FceRI binds IgE molecules with high affinity (K_D of about 10⁻⁹ to 10⁻¹⁰ moles/liter (M)), and can be secreted as a 172-amino acid soluble, IgE-binding fragment by the introduction of a stop codon before the single C-terminal transmembrane anchor; see, for example, Blank et al.,1991, E. J. Biol. Chem. 266, 2639-2646, which describes the secretion of a soluble IgE-binding fragment of 172 amino acids. The extracellular domains of the human FceRIα protein belong to the immunoglobulin (Ig) superfamily and contain seven N-linked glycosylation sites.

Glycosylation of FceRIα affects the secretion and stability of the receptor, but is not required for IgE-binding; see, for example, LaCroix et al., 1993, Mol. Immunol. 30,

321-330; Letourneur et al.,1995, J. Biol. Chem. 270, 8249-8256; Robertson, 1993, J. Biol. Chem. 268, 12736-12743; Scarselli et al., 1993, FEBS Lett 329, 223-226. The beta and gamma chains of FceRI are signal transduction modules.

Prior investigators have disclosed the nucleic acid sequence for human FceRIa; see, for example, U.S. Patent No. 4,962,035, by Leder, issued October 9, 1990; U.S. 5 Patent No. 5,639,660, by Kinet et al., issued June 17, 1997; Kochan et al., 1988, Nucleic Acids Res. 16, 3584; Shimizu et al., 1988, Proc. Natl. Acad. Sci. USA 85, 1907-1911; and Pang et al., 1993, J. Immunol. 151, 6166-6174. Nucleic acid sequences have also been reported for the human FceRI beta and gamma chains; see, respectively, Kuster et al., 1992, J. Biol. Chem. 267, 12782-12787; Kuster et al., 1990, J. Biol. Chem. 265, 10 6448-6452. Nucleic acid sequences have also been reported for nucleic acid molecules encoding canine FceRIa, murine FceRIa, rat FceRIa, feline FceRIa and equine FceRIa proteins; see, respectively, GenBank™ accession number D16413; Swiss-Prot accession number P20489 (represents encoded protein sequence); GenBank accession number J03606; PCT Publication No. WO 98/27208, by Frank et al., published June 25, 1998. 15 referred to herein as WO 98/27208; and PCT Publication No. WO 99/38974, by Weber et al., published August 5, 1999, referred to herein as WO 99/38974. In addition, methods to detect IgE antibodies using a FceRIa protein have been reported in PCT Publication No. WO 98/23964, by Frank et al., published June 4, 1998, referred to 20 herein as WO 98/23964; WO 98/27208, ibid.; PCT Publication No. WO 98/45707, by Frank et al., published October 15, 1998, referred to herein as WO 98/45707; and WO 99/38974, ibid.. WO 98/23964, WO 98/27208, WO 98/45707 and WO 99/38974.

There have been several reports of the use of mutagenesis and swapping techniques to attempt to identify amino acids of either FcεRIα or IgE involved in the binding of (i.e., interaction between) those respective proteins, reports attempting to model FceRIα proteins based on homology to other Ig-superfamily members, and reports that identify compounds that apparently inhibit such binding; see, for example, Cook et al., 1997, Biochemistry 36, 15579-15588; Hulett et al., 1994, J. Biol. Chem. 269, 15287-15293; Hulett et al., 1995, J. Biol. Chem 270, 21188-21194; Mallamaci et al., 1993, J. Biol. Chem. 268, 22076-22083; Robertson, 1993, ibid.; Scarselli et al., 1993, ibid. McDonnell et al., 1997, Biochem. Soc. Trans. 25, 387-392; McDonnell et al.,

10

15

20

25

30

1996, Nat. Struc. Biol. 3, 419-426; PCT Publication No. WO 97/40033, by Cheng et al., published October 30, 1997; U.S. Patent No. 5,180,805, by Gould et al., issued January 19, 1993; U.S. Patent No. 5,693,758, by Gould et al., issued December 2, 1997; PCT Publication No. WO 96/01643, by Gould et al., published January 25, 1996; PCT Publication No. WO 95/14779, by Gould et al., published June 1, 1995. None of these references, however, describe isolated crystals of FcεRIα proteins or 3-D models derived from crystals.

Despite what is known about FcRs and their interaction with antibodies, there remains a need for FcRs with improved characteristics, such as enhanced affinity for antibodies, altered substrate specificity, increased stability, and increased solubility for use in diagnosis, treatment and prevention of allergy and other abnormal immune responses. Also needed for safe and efficacious compounds to prevent or treat allergy and to regulate other immune responses in an animal.

SUMMARY OF THE INVENTION

The present invention includes isolated crystals of the extracellular domains of antibody receptor proteins (FcRs), three-dimensional (3-D) models of such crystals and modifications of such models. The present invention also includes compounds that inhibit the ability of FcRs to bind to antibodies as well as FcR muteins and other modified FcRs. Also included in the present invention are methods to produce and use such crystals, models, inhibitory compounds, muteins, and other modified proteins. As such, the present invention includes FcRs with improved functions such as increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, including but not limited to reduced aggregation. Such proteins, also referred to as muteins, are useful to detect allergy and other in unune response abnormalities as well as to protect an animal from such abnormalities. The present invention also provides safe and efficacious inhibitory compounds to protect (e.g., prevent, treat, reduce the consequences of) an animal from allergy and to regulate other immune responses in an animal.

The present invention includes a 3-D model of an extracellular domain of a human high affinity Fc epsilon receptor alpha chain (FceRIa) protein, wherein the model substantially represents the atomic coordinates specified in Table 1, Table 5, Table 6.

15

20

30

Table 7 or Table 8. The present invention also includes a 3-D model comprising a modification of a model substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8. Also included in the present invention are methods to produce such models.

The present invention also includes an isolated crystal of an extracellular domain of a FceRI\u03c4 protein and methods to produce such a crystal.

The present invention also includes an isolated FcεRIα protein consisting of SEQ ID NO:2 or of SEQ ID NO:4 except that the isoleucine at position 170 is replaced by a cysteine, as well as a protein that is structurally homologous to either such protein. Also included are nucleic acid molecules encoding such proteins, recombinant molecules and recombinant cells including such proteins, and methods to produce such proteins.

The present invention includes a method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein. The method includes the step of using a 3-D model of an extracellular domain of a human FcεRIα protein to identify the compound. Such a model substantially represents the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8. Also included in the present invention are inhibitory compounds identified using such a method. Also included are therapeutic compositions that include such inhibitory compounds and methods to use such therapeutic compositions to protect an animal from allergy or to regulate other immune responses (e.g., protect an animal from other abnormal immune responses).

The present invention also includes a mutein that binds to a Fc domain of an antibody. Such a mutein has an improved function compared to a protein that includes SEQ ID NO:2 or SEQ ID NO:4. Examples of such an improved function include increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, decreased aggregation, and increased solubility. Such a mutein is produced by a method that includes the following steps: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8 to identify at least one amino acid of the protein represented by the model which if replaced by a specified amino acid would effect an improved function of the protein; and (b) replacing the identified amino acid(s) to produce the mutein having such an improved function. The present invention also includes a mutein having an improved

10

15

20

function compared to an unmodified FcεRIα protein, wherein the amino acid sequence of the mutein differs in at least one position from the amino acid sequence of the unmodified protein. Such a position(s) is in at least one of the following regions: a crystal contact cluster, a tryptophan-containing hydrophobic ridge, a FG loop in D2, a D1D2 interface, a cleft between D1 and D2, 2 domain 1, a domain 2, a hydrophobic core, a A'B loop of D1, a EF loop of D1, a BC loop of D2, a C strand of D2, a CC' loop of D2, C'E loop of D2, a strand of D2, the amino terminal five residues of the protein, the carboxyl terminal five residues of the protein, and N-linked glycosylation sites.

Also included are muteins that are chemically modified FceRIa proteins. Also included are nucleic acid molecules that encode muteins of the present invention, recombinant molecules and recombinant cells including such nucleic acid molecules and methods to produce such muteins. Also included are diagnostic reagents and diagnostic kits including such muteins, therapeutic compositions including such muteins, and methods to detect or protect an animal from allergy or other abnormal immune responses.

The present invention also includes a method to improve a function of a FceRIa protein which includes the steps of: (a) analyzing a 3-D model of an extracellular domain of a human high affinity FceRIa protein substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8, to identify at least one amino acid of the protein which if replaced by a specified amino acid improves at least one of the functions of the protein; and (b) replacing the identified amino acid(s) to produce a mutein having at least one of the improved functions.

BRIEF DESCRIPTION OF THE FIGURES

Fig. 1 depicts electron density maps and overall structure of a human FcεRIα model. (A) The 3.0 angstrom experimental electron density map, calculated using the MIRAS phases followed by density modification with the program DM is shown along with a refined model for human FcεRIα. The density is contoured at 1.4σ for residues 147-153. (B) Electron density for carbohydrate moieties linked to N42. The l2Fo-Fcl electron density map, contoured at 1σ, was calculated to 2.4 angstroms using combined MIRAS and model phases (prior to inclusion of carbohydrate in the model). Two N-acetylglucosamines and a mannose moiety were built into the density as shown.

20

25

Fig. 2 depicts a ribbon diagram of a human FcεRIα model showing the positions of the disulfides and the FG loop in domain 2 (D2) that is implicated in receptor specificity. Domain 1 (D1) is shown to the right and D2 is shown to the left.

Fig. 3 depicts a topology diagram of the two domains of a human FcεRIα model showing the hydrogen-bonding patterns of the beta sheet structure. The short stretch of parallel beta-sheet in D1 and D2 caused by the cross-over of the A strand is highlighted. Note that the FG strands of D2 are longer than those of D1, contributing to the prominence of the D2-FG loop.

Fig. 4 demonstrates that a human FcεRIα model has a novel tertiary arrangement of tandem Ig domains.

Fig. 5 depicts sequence alignments of human FcRs. The secondary structure of the two domains is indicated with labeled bars above those residues which form beta-sheet in FceRI. Below the sequences, carbohydrate attachment sites found in seventeen different FcR sequences are indicated with a (+). This analysis is based on the seven human receptors shown and the non-human receptors listed in Table 4.

Fig. 6 depicts the four surface-exposed tryptophans at the top of the D2 domain of a human FcεRIα model that are implicated in IgE binding.

Fig. 7 depicts residues in the D2 FG loop and D1 E strand of a human FcεRIα model that are highly variable in human FcR sequences. The residues in the D2-FG loop have been directly implicated in IgE binding. The residues in the D1 E strand and the D1 A'B loop are located near the top of the D2 domain and could form part of an extended IgE-binding surface between the two domains.

Fig. 8 depicts a juxtaposition of a human FcεRIα model with a model for the intact IgE antibody structure. The insertion of the Cε2 domains in the IgE molecule are indicated by dotted lines. The FcεRIα protein is shown relative to the mast cell membrane near the top of the Cε3 domains that bind to the receptor.

DETAILED DESCRIPTION OF THE INVENTION

The present invention includes isolated crystals of the extracellular domains of FcRs, 3-D models of such crystals and modifications of such models. The present invention also includes compounds that inhibit the ability of FcRs to bind to antibodies as well as muteins and other modified FcRs. Also included in the present invention are

20

methods to produce and use such crystals, models, inhibitory compounds, muteins, and other modified proteins.

The present invention includes an isolated crystal of an extracellular domain of a high affinity Fc epsilon receptor alpha chain (FceRIa), a 3-D model of such a crystal and a modification of such a model. As used herein, the term "a" entity or "an" entity refers to one or more of that entity; for example, a crystal or a model refers to one or more crystals or models, respectively. As such, the terms "a" (or "an"), "one or more" and "at least one" can be used interchangeably herein. It is also to be noted that the terms "comprising", "including", and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures, or combinations, of two or more of the compounds.

As used herein, an extracellular domain of a Fc ϵ RI α protein is the portion of the FceRI alpha chain that is exposed to the environment outside the cell and that binds to the Fc domain of an IgE antibody. Such an extracellular domain can be (a) a complete extracellular domain which is a domain that extends from the first amino acid of a mature FceRI alpha chain through the last amino acid prior to the start of the transmembrane region or a domain that is functionally equivalent, in that such a domain includes a D1 and D2 domain, displays a similar affinity for the IgE antibody to which such an FcεRIα protein naturally binds, and produces crystals having sufficient quality to enable structure determination, or (b) a fragment of any of the extracellular domains of (a), wherein the fragment retains its ability to bind to the Fc domain of an antibody. As used herein, the terms binding to an antibody and binding to the Fc domain (i.e., constant region) of an antibody can be used interchangeably since it is recognized that a FcR binds to the Fc domain of an antibody. A FcR (i.e., a protein that can bind to an antibody), such as a FceRIa protein, can be a full-length FcR (e.g., a full-length FceRI alpha chain), or any fragment thereof, wherein the fragment binds to an antibody. Similarly an antibody, or an Fc domain thereof, can be a full-length antibody, or fulllength Fc domain thereof, or any fragment thereof that binds to a FcR. Preferably a FcR binds to an antibody with an affinity (K_A) of at least about 10⁸ liters/mole (M⁻¹), more 30 preferably of at least about 10° M⁻¹, and even more preferably of at least about 10¹⁰ M⁻¹.

The present invention is surprising in several aspects. For example, this is the first report of an isolated crystal of an extracellular domain of a FcεRIα protein, and in particular of an isolated crystal of sufficient quality that a crystal structure, i.e., a 3-D model, could be derived therefrom. The inventors believe that this protein also represents the most highly glycosylated protein for which a crystal and a 3-D model have been reported to date. Not only does glycosylation interfere with protein crystal formation but it also is difficult to consistently produce recombinant proteins having a uniform glycosylation pattern. Generation of such a crystal was very difficult and nonobvious and has been attempted by others without success. The inventors tried many approaches before discovering that a preferred FceRIa protein from which to make a useful crystal is a FceRIa protein that consists of amino acids 1 through 176 of the mature human FceRIa protein. This protein is denoted herein as PhFceRIa₁₋₁₇₆, or the hFcεRIα₁₋₁₇₆ protein, and has an amino acid sequence denoted herein as SEQ ID NO:2. An example of a nucleotide acid molecule encoding PhFceRIa₁₋₁₇₆ is referred to herein as nhFceRIa₁₋₅₂₈, the nucleic acid sequence of which is denoted herein as SEQ ID NO:1. It was also discovered that better crystals are generated when PhFcεRIα₁₋₁₇₆ is produced in insect cells, using a method such as that described in the Examples. Determination of the crystal structure of PhFceRIa₁₋₁₇₆ produced in Trichoplusia ni (Hi-5) cells resulted in a 3-D model that substantially represents the atomic coordinates specified in Table 1, referred to herein as form M1. Amino acids are represented herein by their standard 20 three or one letter codes; see, for example, Sambrook et al., Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Labs Press, 1989. Prior to obtaining a crystal of sufficient quality to solve its crystal structure using insect-cell produced PhFceRI α_1 176, a number of other proteins were tried, including a FceRIa protein spanning from amino acid 1 through 171 of SEQ ID NO:2 produced in Pichia pastoris, and FceRIa 25 proteins spanning from amino acid 1 through 172 of SEQ ID NO:2 produced in Chinese hamster ovary cells, Trichoplusia ni cells, and Spodoptera frugiperda cells without success. Without being bound by theory, it is believed that PhFceRIa₁₋₁₇₆ was a better candidate because it apparently represents a complete extracellular domain. Based on the 3-D model of PhFceRI α_{1-176} , the inventors believe, without being bound by theory, that the amino acid at position 172 is important in the structure determination and that,

-10-

in order to form a crystal of sufficient quality to determine the first 3-D model of a FceRIa protein, at least one additional amino acid was required carboxyl-terminal to that at position 172; the inventors further believe that an optimal protein would span from the amino acid at position 3 through the amino acid at position 174 of SEQ ID NO:2. It should be noted, however, that having solved the crystal structure of a first $Fc\epsilon RI\alpha$ protein enables the solving of crystal structures of additional FcεRIα proteins as well as of additional FcRs in general. For example, the crystal structures of two additional crystals cited in the Examples can be solved using a combination of X-ray diffraction data of the crystals per se and information derived from the 3-D model of PhFc ϵ RI α_{1-176} . The examples also describe the solution of an additional four crystal structures using such information, namely the examples present 3-D models of: (a) a human FcεRIα 10 protein spanning amino acids 1-172 of SEQ ID NO:2 (i.e., PhFceRIa₁₋₁₇₂, the amino acid sequence of which is represented herein as SEQ ID NO:4) expressed in lec1 Chinese hamster ovary (CHO) cells, the structural form being referred to herein as Form T1; (b) a second structural form of PhFc ϵ RI α_{1-172} produced in lec1 CHO cells, referred to herein as Form T2; (c) a second structural form of a PhFceRIa₁₋₁₇₆ protein expressed in T. ni (Hi5) 15 cells, referred to herein as Form M2; and (d) a PhFc ϵ RI α_{1-172} protein in which the isoleucine at position 170 of SED ID NO:4 is replaced with a cysteine, expressed in Sf9 insect cells, a structural form referred to herein as H1. The atomic coordinates of the crystal structural forms T1, T2, M2 and H1 are presented, respectively, in Tables 5, 6, 7, 20 and 8.

The 3-D model of the hFc ϵ RI α_{1-176} protein form M1 is also very surprising in view of the knowledge of the structure of proteins containing immunoglobulin domains, herein also referred to as Ig domains. The most striking differences, which are described in greater detail below, include, but are not limited to: domain 1 (D1) and domain 2 (D2) of the model of PhFc ϵ RI α_{1-176} are much smaller than known Ig domains; the packing and 25 orientation of D1 and D2 of the hFcεRIα₁₋₁₇₆ protein are significantly different from known Ig domain-containing proteins in that, for example, the bend angle between D1 and D2 of the PhFceRI α_{1-176} structure is much more acute than for other proteins, the relative rotational orientation of the two domains is much different, D1 and D2 of PhFceRI α_{1-176} form an unusual interface and cleft, D1 and D2 of PhFceRI α_{1-176} are

antiparallel, the presence of a hydrophobic surface on the two faces of the model of PhFcεRIα₁₋₁₇₆ which appear to be nearby or directly involved in binding to IgE antibodies; the FG loop of D2 of PhFceRI α_{1-176} , also apparently involved in binding to IgE antibodies, projects much more significantly above the D2 domain than is seen for known D2-containing proteins; and the interruption in structure between strands A and A' in D1 which apparently leads to interaction between the two domains. It is to be noted that although most known Ig domain pairs which are parallel, some Ig domains are antiparallel (e.g., hemolin) but the domain:domain orientation and specifics of packing of those domains are very different from the orientation and packing of PhFceRI α_{1-176} . It is also surprising that the model of the hFc ϵ RI α_{1-176} protein predicts that an IgE antibody interacts with D1 as well as D2 in view of the mutagenesis analysis studies conducted to date all of which have only identified mutations in D2 that lead to decreased, or increased, binding between a FceRIa protein and an IgE antibody. As such, a model of the present invention is necessary for proper interpretation and refinement of mutagenesis and region swapping studies that have been reported. Such a model for the first time permits the differentiation between amino acids directly or indirectly influencing binding of IgE to FceRIa and demonstrates where amino acids and amino acid segments identified in mutagenesis and swapping studies are positioned on the protein. It is to be noted that the 3-D models of FceRIa crystal structure forms T1, T2, M2 and H1 are quite similar to that of form M1, with the following differences. The principal differences in the structures from the various crystal forms occur in the BC 20 loop in domain 1 (the "30 loop"), the C' strand in domain 2 (the "130 region") and the carbohydrate sites. There are also smaller differences in the termini of the structures and the FG loop in domain 1 (the "72 loop"). These differences are described in more detail in the Examples. 25

One embodiment of the present invention is an isolated crystal of an extracellular domain of a FccRI\alpha protein. As used herein, an isolated crystal is a crystal of a protein that has been produced in a laboratory; that is, an isolated crystal is produced by an individual and is not an object found in situ in nature. It is appreciated by those skilled in the art that there are a variety of techniques to produce crystals including, but not limited to, vapor diffusion using a hanging or sitting drop methodology, vapor diffusion

30

under oil, and batch methods; see, for example, Ducruix et al., eds., 1991, Crystallization of nucleic acids and proteins; A practical approach, Oxford University Press, and Wyckoff et al., eds., 1985, Methods in Enzymology 11, 49-185. It is also to be appreciated that crystallization conditions can be adjusted depending on a protein's inherent characteristics as well as on a protein's concentration in a solution and that a variety of precipitants can be added to a protein solution in order to effect crystallization; such precipitants are known to those skilled in the art. In a preferred embodiment, a crystal of a FceRIa protein is produced in a solution by adding a precipitant such as polyethylene glycol (PEG) or PEG monomethylether. In a particularly preferred embodiment, the precipitant PEG is added to .. solution to achieve a final concentration of from about 10 percent (%) to about 40%, preferably from about 12% to about 32% PEG per volume solution. It is also to be noted that a FcεRIα protein used to produce a crystal can be produced by a variety of methods, including purification of a native protein, chemical synthesis of a protein, or recombinant production of a protein. Although a number of cell types can be used to recombinantly produce such a protein, insect cells, such as, but not limited to Trichoplusia ni and Spodoptera frugiperda, are preferred, with Trichoplusia ni cells being more preferred. Also preferred are Chinese hamster ovary cells. Additional methods to produce proteins are disclosed below.

Isolated crystals of the present invention can include heavy atom derivatives, such as, but not limited to, gold, platinum, mercury, selenium, and lead. Such heavy atoms can be introduced randomly or introduced in a manner based on knowledge of 3-D models of the present invention. Additional crystals of the present invention are not derivatized. In one embodiment, an isolated crystal of the present invention is a co-crystal of a FceRIα protein bound to a Fc domain of an IgE antibody. In another embodiment, an isolated crystal of the present invention is a co-crystal of a FceRIα protein and a compound that inhibits the binding of a FceRIα protein to a Fc domain of an IgE antibody. Additional crystals of the present invention include crystals produced from proteins that are muteins of the present invention or other proteins that are represented by a 3-D model of the present invention.

An isolated crystal of the present invention can be the crystal of any suitable extracellular domain of a FceRI\alpha protein. Suitable FceRI\alpha proteins include mammalian

FceRIa proteins, with human, canine, feline, equine, rat and murine FceRIa proteins being preferred, and human FceRIa proteins being even more preferred. A preferred crystal of the present invention diffracts X-rays to a resolution of about 4.0 angstroms or higher (i.e., lower number meaning higher resolution), with resolutions of about 3.5 angstroms or higher, about 3 angstroms or higher, about 2.5 angstroms or higher, about 2 angstroms or higher, about 1.5 angstroms or higher, and about 1 angstrom or higher being increasingly more preferred. It is appreciated, however, that additional crystals of lower resolutions can have utility in discerning overall topology of the structures, e.g., location of a binding site or where a molecule binds to a receptor. A particularly preferred isolated crystal of the present invention has the amino acid 10 sequence SEQ ID NO:2, amino acid sequence SEQ ID NO:4, or a sequence essentially equivalent that represents an extracellular domain of another mammalian $FceRI\alpha$ protein. SEQ ID NO:4 is the amino acid sequence of a protein consisting of the first 172 residues of a mature human FcεRIα protein denoted herein as PhFcεRIα₁₋₁₇₂; i.e., SEQ ID NO:4 spans from amino acid residue 1 through amino acid residue 172 of SEQ ID 15 NO:2. An example of a nucleotide acid molecule encoding PhFc ϵ RI α_{1-172} is referred to herein as nhFceRIa₁₋₅₁₆, the nucleic acid sequence of which is denoted herein as SEQ ID NO:3. Preferred are crystals that belong to monoclinic space group C2 or monoclinic space group P6122. Particularly preferred crystals include: a crystal of PhFceRI α_{1-176} that belongs to monoclinic space group C2, has cell dimensions of 88.6 angstroms x 69.6 angstroms x 49.3 angstroms, alpha=gamma=90.0 degrees, beta=116.69 degrees, and diffracts X-rays to a resolution of about 2.4 angstroms (form M1); a crystal of PhFceRI α_{1-176} that belongs to monoclinic space group C2, has cell dimensions of 136.02 angstroms x 75.01 angstroms x 79.28 angstroms, alpha=gamma=90 degrees, beta=117.8 degrees, and diffracts X-rays to a resolution of about 3.0 angstroms; and a crystal of 25 PhFceRI α_{1-172} that belongs to monoclinic space group P6122, has cell dimensions of 58 angstroms x 58 angstroms x 226 angstroms, alpha=beta=90 degrees, gamma=120 degrees, and diffracts X-rays to a resolution of about 3.2 angstroms. Also preferred crystals include: a crystal of PhFceRIa₁₋₁₇₂ that belongs to tetragonal space group P4₃, has cell dimensions of 145.08 angstroms x 145.08 angstroms x 62.74 angstroms, 30 alpha=beta=gamma=90.0 degrees, and diffracts X-rays to a resolution of about 3.1

angstroms (form T1); a crystal of PhFcεRIα₁₋₁₇₂ that belongs to tetragonal space group
P4₃, has cell dimensions of 150.50 angstroms x 150.50 angstroms x 74.18 angstroms,
alpha=beta=gamma=90.0 degrees, and diffracts X-rays to a resolution of about 3.8
angstroms (form T2); a crystal of PhFcεRIα₁₋₁₇₆ that belongs to monoclinic space group
C2, has cell dimensions of 136.90 angstroms x 73.79 angstroms x 79.40 angstroms,
c3. P model of an extracellular domain of a

The present invention includes a 3-D model of an extracellular domain of a FcεRIα protein that substantially represents the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8. The present invention also includes 3-D models that comprise modifications of the model substantially represented by the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8. Each such modification represents a protein that binds to a Fc domain of an antibody. A 3-D model of an extracellular domain of a FceRIa protein is a representation, or image, that predicts the actual structure of the corresponding protein. As such, a 3-D model is a tool that can be used to probe the relationship between the protein's structure and function at the atomic level and to design muteins (i.e., genetically and/or chemically altered FcRs) having an improved function, such as, but not limited to: increased (i.e., enhanced) 20 stability; increased antibody binding activity, for example, by, increasing the affinity for an antibody by, for example, increasing the association rate and/or decreasing the dissociation rate between a FcR and an antibody or by altering substrate specificity (e.g., enhancing the ability of a FcR of a certain species and class to bind to antibody from another species and/or another antibody class); and/or increased solubility (e.g., reduced 25 aggregation). It is well known to those skilled in the art, however, that a 3-D model of a protein derived by analysis of protein crystals is not identical to the inherent structure of the protein. See, for example, Branden et al., Introduction to Protein Structure, Garland Publishing Inc., New York and London, 1991, especially on page 277, which states "not surprisingly the model never corresponds precisely to the actual crystal." Furthermore, 30

the model can be subjected to further refinements to more closely correspond to the actual structure of a FcR. Such a refined model, which is an example of a modification of the present invention, is a better predictor of the actual structure and mechanism of action of the protein that the model represents. A refinement of a 3-D model of the present invention refers to an improved model of a FcεRIα protein that can be obtained in a variety of ways known to those skilled in the art. Refinements can include models determined to more preferred degrees of resolution, preferably to about 3.5 angstroms, more preferably to about 2 angstroms, more preferably to about 2.5 angstroms, and even more preferably to about 2 angstroms, more preferably to about 1.5 angstroms, and even more preferably to about 1 angstrom. Preferred refinements are obtained using the 3-D model as a basis for such improvements.

One embodiment of the present invention is a 3-D model of an extracellular domain of a FceRIa protein that substantially represents the atomic coordinates specified (i.e., listed) in Table 1.

Table 1. Atomic coordinates of PhFceRIa₁₋₁₇₆, Form M1

ATOM NUMBER	ATOM TYPE	RESIDUE	_#_	_ <u>x</u> _	<u>Y</u>		occ	_B_
5 2 3	CB CG	LYS LYS LYS LYS	4 4 4	23.345 23.455 23.900 24.017	19.877 20.034 21.444 21.633	27.253 25.744 25.387 23.885 23.539	1.00 1.00 1.00 1.00 1.00	114.16 114.16 114.16 114.16 114.16
4 5 6 10 7 8	CE NZ C O N	LYS LYS LYS LYS LYS	4 4 4 4	24.406 23.899 24.999 22.817 22.920	23.028 17.439 17.777 18.457 18.482	27.171 26.726 29.211 27.721 27.224	1.00 1.00 1.00 1.00 1.00	98.73 98.73 98.73 98.73 89.31
9 10 11 15 12 13	CA N CD CA CB	PRO PRO PRO PRO PRO	5 5 5 5	23.522 22.385 24.397 23.912 22.445	16.148 15.565 15.093 13.858 14.102	27.963 26.708 27.454 27.562 25.190	1.00 1.00 1.00 1.00 1.00	81.52 89.31 81.52 81.52 89.31
14 15 16 20 17 18	CG C O N CA	PRO PRO LYS LYS	5 5 6 6	24.212 23.503 24.844 24.719 25.816	14.980 15.784 13.992 13.835 14.639	24.581 24.575 23.137 22.433	1.00 1.00 1.00 1.00 1.00	89.31 79.33 79.33 122.37 122.37
19 20 21 25 22 23	CB CG CD CE NZ	LYS LYS LYS LYS LYS	6 6 6	25.411 26.324 25.774 26.602 24.794	15.180 16.320 17.040 18.225 12.368	21.073 20.643 19.421 19.060 22.740	1.00 1.00 1.00 1.00	122.37 122.37 122.37 79.33 79.33
24 25 26 30 27 28	C O N CA CB	LYS LYS VAL VAL VAL	6 7 7 7	25.644 23.884 23.879 22.479 22.530	11.622 11.948 10.567 10.128 8.711	23.231 21.866 21.409 20.951 20.408	1.00 1.00 1.00 1.00	65.03 65.03 74.25 74.25 74.25
29 30 31 35 32	CG: CG: C O N		7 7 7 7 8	21.515 24.846 24.829 25.713	10.205 10.463 11.290 9.462 9.255	22.113 20.24 19.32 20.29 19.23	4 1.00 B 1.00 9 1.00	65.03 65.03 46.54 46.54
33 34 35 36 40 37	CA CB OC C	SER SER SER SER	8 8 8 8	26.517	9.513 8.670 7.815 6.955	19.74 20.83 18.78 19.56 17.51	.9 1.00 .6 1.00 .60 1.00 .67 1.00	64.02 46.54 46.54
38 39 40 41 45 42	0 2 0 0 0	A LEU B LEU G LEU	999	26.840 26.674 25.796 24.620	7.556 6.227 6.283 6 7.256	16.94 15.6 15.5 14.3	45 1.00 79 1.00 29 1.0 38 1.0	55.36 0 45.99 0 45.99 0 45.99
43 44 45 46	С	D1 LEU D2 LEU LEU LEU ASI)) N	9 23.78 9 27.98 9 28.89 10 28.06	7.246 3 5.585 4 6.250 4.274	16.7 16.5 16.0 16.7 16.3	555 1.0 991 1.0 713 1.0 318 1.0	55.36 55.36 50 55.82 50 52.82
50 47 48 49 50	(DA ASI DB AS DG AS DD1 AS	N N N N	10 29.24 10 30.17 10 31.36 10 32.03 10 31.6	3.353 66 2.495 32 2.717 45 1.504	17.! 17. 16. 18.	510 1.0 166 1.0 155 1.0 004 1.	00 77.87 00 77.87 00 77.87 00 52.82
55 52 53 54 55 56	,	C AS O AS N PF CD PI	SN SN RO RO	10 28.8 10 28.3 11 28.9 11 28.7 11 29.5	20 1.361 166 2.024 155 0.707 503 2.975	16. 14. 13 5 13	.492 1. .432 1. .793 1 .454 1	00 52.82 00 54.26 .00 46.78 .00 54.26 .00 46.78
60 57 58			RO RO	11 29.5	512 2.179	, 12	1.155 1	

59	CG C		11	29.707 28.692	0.774 4.268	12.631 13.348 13.775	1.00 1.00 1.00	46.78 54.26 54.26
60	0	PRO	11	27.541	4.332	12.742	1.00	56.88
61	N .	PRO	12	29.286	5.303 5.189	12.120	1.00	56.23
62 5 63	CD	PRO	12	30.615	6.646	12.514	1.00	56.88
64	CA	PRO	12	28.751 29.888	7.348	11.788	1.00	56.23
65	CB	PRO	12 12	31.093	6.592	12.191	1.00	56.23
66	CG	PRO	12	27.458	6.798	11.736	1.00	56.88 56.88
67	C	PRO PRO	12	26.680	7.710	12.003	1.00 1.00	54.29
10 68	0	TRP	13	27.255	5.930	10.751 9.881	1.00	54.29
69	N CA	TRP	13	26.079	5.991	8.794	1.00	47.07
70 71	CB	TRP	13	26.203	4.929 4.697	8.423	1.00	47.07
71 72	CG	TRP	13	27.629 28.502	5.622	7.767	1.00	47.07
15 73	CD2	TRP	13	29.762	4.998	7.659	1.00	47.07
74	CE2	TRP	13 13	28.341	6.919	7.266	1.00	47.07 47.07
75	CE3	TRP TRP	13	28.372	3.584	8.676	1.00 1.00	47.07 47.07
76	CD1 NE1	TRP	13	29. 65 5	3.756	8.218 7.064	1.00	47.07
77	CZ2	TRP	13	30.853	5.62	6.679	1.00	47.07
20 78 79	CZ3	TRP	13	29.419	7.536 6.890	6.582	1.00	47.07
80	CH2	TRP	13	30.664	5. 83 6	10.602	1.00	54.29
81	С	TRP	13	24.753 24.571	4.912	11.389	1.00	54.29
82	0	TRP	13 14	23.838	6.759	10.323	1.00	44.90
25 83	N	ASN ASN	14	22.513	6.758	10.925	1.00 1.00	44.90 62.66
84	CA	ASN	14	22.099	8.179	11.291	1.00	62.66
85	CB CG	ASN	14	21.713	8.992	10.083 9.152	1.00	62.66
86 87	OD1	ASN	. 14	22.501	9.154 9.505	10.085	1.00	62.66
87 30 88	ND2	ASN	14	20.489	6.158	9.935	1.00	44.90
89	C	ASN	14	21.504 20.302	6.059	10.229	1.00	44.90
90	0	ASN	14 15	22.006	5.777	8.759		43.26 43.26
91	N.	ARG ARG	15	21.189	5.130	7.735		51.24
92	CA	ARG	15	21.196	5.926	6.426 6.623		51.24
35 93	CB CG	ARG	15	21.031	7.419	5.311		51.24
94 95	CD	ARG	15	21.112	8.161 8.119	4.637		51.24
96	NE	ARG	15	19.813	7.770	3.37	5 1.00	51.24
97	CZ	ARG	15	19.648 20.693	7.441	2.65		51.24
40 98	NH1	ARG	15 15		7.743	2.84		51.24 43.26
99	NH2	ARG ARG	15		3.799	7.54	5 1.00 1 1.00	43.26
100	C	ARG	15		3.759	7.03 7.98	_	47.47
101	0 N	ILE	16	21.258	2.719	7. 9 0 7.89		47.47
102 45 103	CA	ILE	16		1.386 0.864	9.30		38.74
104	CB	ILE	16		1.866	10.02	26 1.00	38.74
105	CG2		16		0.673	10.13	39 1.00	38.74 38.74
106	CG1		10	4-4	0.154	11.50		47.47
107	CD1	ILE ILE	10	6 20.912	0.357	7.2		47.47
50 108	C	ILE	1	6 19.711	0.579	7.1° 6.9	• •	45.27
109 110	Ň	PHE		7 21.480		6.3		45.27
111	CA	PHE		7 20.721		5.4		33.04
112	СВ	PHE		7 21.636 7 21.911	40	4.1	13 1.00	
55 113	CG			7 21.911 7 23.185		3.5		
114	CD.			7 20.864	-1.725		322 1.00	
115	CD			7 23.432	-1.782		307 1.00 036 1.00	1
116	CE:	·		17 21.106	3 -1.272		036 1.00 523 1.00	
60 118			•	17 22.38			334 1.00	45.27
119	_	PHE		17 20.02			433 1.00) 45.27
120	0	PHE		17 20.544 18 18.84	40		959 1.0	48.86
121	N	LYS		18 18.84 18 18.07		_	806 1.0	48.86
122		LYS		,5 ,5,5,				

							7.005	1.00	55.91
		СВ	LYS	18 -	16.848	-4.630 - 5.004			55.91
	123	CG		18	16.039	-5.694 -5.696			55.91
	124 125	CD	LYS		14.629	-6.718		1.00	55.91
	126	CE .	LYS	18	13.744 13.936	-8.075	7.298	1.00	55.91
5	127	NZ	LYS	18	19.003	-5.299	8.149	1.00	48.86 48.86
_	128	С	LYS	18 18	19.635	-5.875	7.267	1.00	53.46
	129	0	LYS GLY	19	19.106	-5.627	9.429	1.00 1.00	53.46
	130	N	GLY	19	19.993	-6.705	9.832 10.311	1.00	53.46
10	131	CA C	GLY	19	21.381	-6.284 7.117	10.837	1.00	53.46
10	132 133	ŏ	GLY	19	22.111	-7.117 -5.016	10.134	1.00	46.04
	134	Ň	GLU	20	21.758 23.073	-4.533	10.576	1.00	46.04
	135	CA	GLU	20	23.553	-3.372	9.700	1.00	45.53 45.53
	136	CB	GLU	20 20	23.544	-3.671	8.197	1.00 1.00	45.53 45.53
15	137	CG	GLU GLU	20	24.253	-2.611	7.347 7.587	1.00	45.53
	138	CD OE1	GLU	20	24.049	-1.393	6.423	1.00	45.53
	139	OE2	ĞĹÜ	20	25.008	-3.004 -4.083	12.039	1.00	46.04
	140 141	C	GLU	20	23.046	-3.958	12.654	1.00	46.04
20	142	Ū	GLU	20	21.980 24.223	-3.845	12.607	1.00	50.99
20	143	N	ASN	21 21	24.223	-3.422	13.994	1.00	50.99 67.08
	144	CA	ASN ASN	21	25.255	-4.321	14.790	1.00 1.00	67.08
	145	CB	ASN	21	24.817	-5.776	14.825 15.049	1.00	67.08
۰.	146	CG OD1	ASN	21	23.634	-6.077	14.619	1.00	67.08
25	147	ND2	ASN	21	25.782	-6.675 -1.985	14.118	1.00	50.99
	148 149	C	ASN	21	24.765	-1.493	13.290	1.00	50.99
	150	0	ASN	21	25.5 3 3 24.291	-1.317	15.164	1.00	48.02 48.02
	151	N	VAL	22 22	24.674	0.058	15.453	1.00 1.00	39.09
30		CA	VAL VAL	22	23.752	1.086	14.742 15.215	1.00	39.09
	153	CB CG1	VAL	22	22.313	0.924	15.023	1.00	39.09
	154	CG2	VAL	22	24.243	2.499 0.241	16.964	1.00	48.02
	155 156	C	VAL	22	24.552	-0.203	17.577	1.00	48.02
35	5 157	0	VAL	22	23.568 25.558	0.870	17.570	1.00	52.73
٥.	158	N	THR	23 23	25.530	1.102	19.013	1.00	52.73 65.60
	159	CA	THR THR	23	26.848	0.666	19.686 19.570		65.60
	160	CB OG1	THR	23	26.999	-0.754	21.162		65.60
4	161 0 162	CG2	THR	23	26.849	1.059 2.577	19.294	1.00	52.73
4	163	C	THR	23	25.313 25.946	3.422	18.673	1.00	52.73
	164	0	THR	23 24		2.883	20.214		47.77 47.77
	165	N	LEU LEU	24		4.267	20.576		58.94
	166	CA	LEU	24		4.561	20.543 19.303		58.94
4	15 167	CB CG	LEU	24	21.813	4.200	19.40		58.94
	168 169	CD1	LEU	24		4.824 4.704	18.06		58.94
	170	CD2	LEU	24		4.528	21.98	0 1.00	47.77
	171	С	LEU	24 24		3.858	22. 9 5		47.77 57.92
	50 172	0	LEU	2		5.510	22.08		57.92
	173	N	THR THR	2	5 26.155	5.867	23.37 23.31		61.52
	174	CA CB	ن، با	2	5 27.70 0	5.784	22.99		61.52
	175 176	OG.		2			24.60		61.52
	55 177	CG	2 THR		5 28.292		23.8		57.92
	178	С	THR		25.738 25.732		23.0		
	179	0	THR		25.732 26 25.397	7.394	25.1	01 1.00	
	180	N	CYS		26 24.998	3 8.662	25.6		
	181	CA	CYS		26 26.319	9.363	26.0 26.2		
	60 182	CO	CYS	:	26 27.330		26.2 26.9		68.33
	183 184		CYS	1	26 24.14		27.5	559 1.00	68.33
	185		i CYS		26 23.11 27 26.31		26.0		
	186		ASN	l	27 26.31				

	187	CA CB	ASN ASN	27 27	27.538 27.183	11.474 12.865	26.307 26.803		98.51 123.41 123.41
	188 189	CG .	ASN	27	27.922	13.945	26.038 25.618		123.41
	190	OD1	ASN	27	29.067	13.760 15.085	25.851		123.41
	191	ND2	ASN	27	27.268 28.671	10.911	27.174	1.00	98.51
	192	С	ASN	27 27	28.481	9.968	27.937	1.00	98.51
	193	0	ASN GLY	28	29.849	11.531	27.053	1.00	112.08
	194	N CA	GLY	28	31.050	11.111	27.774	1.00	112.08 112.08
10	195	C	GLY	28	31.283	11.487	29.235 29.874	1.00 1.00	112.08
10	196 197	ŏ	GLY	28	32.175	10.929	29.772	1.00	117.67
	198	Ň	ASN	29	30.513	12.430 12.818	31.175	1.00	117.67
	199	CA	ASN	29	30.674 30.018	14.176	31.464	1.00	132.23
	200	CB	ASN	29 29	30.579	15.301	30.619	1.00	132.23
15	201	CG	ASN ASN	29	31.792	15.505	30.559	1.00	132.23 132.23
	202	OD1 ND2	ASN	29	29.693	16.049	29.971	1.00 1.00	117.67
	203 204	C	ASN	29	30.009	11.779	32.077 33.277	1.00	117.67
	205	ŏ	ASN	29	30.259	11.737 10.943	31.489	1.00	110.72
20	206	N	ASN	30	29.158 28.423	9.921	32.235	1.00	110.72
	207	CA	ASN	30	27.236	9.430	31.395	1.00	135.09
	208	СВ	ASN	30 30	26.331	8.468	32.153	1.00	135.09
	209	CG	ASN ASN	30	26.684	7.989	33.231	1.00	135.09 135.09
0.5	210	OD1 ND2	ASN	30	25.163	8.183	31.590	1.00 1.00	110.72
25	211	C	ASN	30	29.267	8.721	32.680 31.853	1.00	110.72
	212 213	ŏ	ASN	30	29.834	8.000	33.995	1.00	129.04
	214	Ň	PHE	31	29.338	8.509 7.397	34.559	1.00	129.04
	215	CA	PHE	31	30.095 31.178	7.900	35.519	1.00	95.73
30	216	CB	PHE	31	32.321	8.589	34.837	1.00	95.73
	217	CG	PHE PHE	31 31	32.106	9.716	34.059	1.00	95.73
	218	CD1 CD2	PHE	31	33.619	8.127	34.993	1.00	95.73 95.73
	219	CE1	PHE	31	33.166	10.380	33.440	1.00 1.00	95.73
35	220 221	CE2	PHE	31	34.687	8.784	34.378 33.603	1.00	95.73
20	222	CZ	PHE	31	34.458	9.915 6.440	35.308	1.00	129.04
	223	C	PHE	31	29.181	6.850	35.908	1.00	129.04
	224	0	PHE	31 32	28.188 29.531	5.160	35.260	1.00	141.76
	225	N.	PHE PHE	32 32	28.775	4.109	35.937	1.00	141.76
40		CA	PHE	32	29.529	2.765	35.876	1.00	141.76 141.76
	227	CB CG	PHE	32	30.787	2.788	35.031 35.280	1.00 1.00	141.76
	228 229	CD1	PHE	32	31.814	3.706	33.260	1.00	141.76
	230	CD2	PHE	32	30.953	1.870 3.712	34.501	1.00	141.76
45		CE1	PHE	32	32.985	1.867	33.209		141.76
	232	CE2	PHE	32 32		2.787	33.464	1.00	141.76
	233	CZ	PHE PHE	32		4.481	37.408		141.76
	234	C	PHE	32		5.140	38.017		141.76 141.76
50	235	O N	GLU	33	27.433	4.055	37.969		141.76
3(0 236 237	CA	GLU	33		4.330	39.369 40.292		141.76
	238	CB	GLU	33		3.831 2.332	40.22	-	141.76
	239	CG	GLU	33		1.496	40.51		141.76
	240	CD	GLU	33 33		2.073	40.92		141.76
5	5 241	OE1	GLU	3		0.256	40.34		141.76
	242	OE2	GLU	3		5.802	39.68		141.76 141.76
	243	CO	GLU	3	3 26.382	6.125	40.80		137.33
	244 245	Ň	VAL	3	4 26.967	6.689	38.70 38.89		137.33
6	50 246	CA	VAL	3	100		37.87		109.45
	247	СВ	VAL		4 27.428	4-444	37. 9 7		109.45
	248	CG1			4 26.940 4 28.929		38.14	0 1.00	
	249	CG2	VAL		14 28.929 14 25.167		38.63		
	250	С	VAL	•	., 201101				

					~4 000	8.503	39.545		137.33
	251	0	VAL	•	24.368	8.021	37.375	1.00	141.76
	252	Ñ	SER		24.807	8.110	36.909	1.00	141.76
	253	CA	SER	35	23.432	9.522	36.351	1.00	133.69
	254 ·	CB	SER	35	23.189	9.652	35.667	1.00	133.69
	255 255	OG	SER	35	21.955	7.055	35.828	1.00	141.76
	256	C	SER	35	23.164	7.036	34,785	1.00	141.76
	257	0	SER	35	23.825 22.226	6.148	36.087	1.00	88.62
	258	N	SER	36		5.151	35.080	1.00	88.62
	259	CA	SER	36	21.891 20.818	4.198	35.591	1.00	92.65
10	260	CB	SER	36	19.623	4.905	35.850	1.00	92.65
10	261	OG	SER	36	21.335	6.012	33.959	1.00	88.62
	262	С	SER	36	20.928	7.150	34.193	1.00	88.62
	263	0	SER	36	21.332	5.495	32.741	1.00	66.50
	264	N	THR	37 37	20.833	6.279	31.625	1.00	66.50
15	265	CA	THR	37 37	21.718	6.049	30.395	1.00	64.10
	266	CB	THR	37	23.085	6.313	30.748	1.00	64.10
	267	OG1	THR	37	21.299	6.969	29.254	1.00	64.10
	268	CG2	THR	37	19.369	6.003	31.268	1.00	66.50
	269	C	THR THR	37	18.855	4.912	31.478	1.00	66.50 59.63
20	270	0	LYS	38	18.693	7.025	30.764	1.00	59.63
	271	N	LYS	38	17.304	6.899	30.331	1.00	48.08
	272	CA	LYS	38	16.430	7.945	31.017	1.00	48.08
	273	CB	LYS	38	15.696	7.418	32.220	1.00	48.08
	274	CG	LYS	38	15.075	8.535	33.017	1.00	48.08
25	275	CD CE	LYS	3ხ	14.471	7.971	34.289	1.00 1.00	48.08
	276	NZ	LYS	38	13.893	9.058	35.108	1.00	59.63
	277	C	LYS	38	17.274	7.120	28.820	1.00	59.63
	278	Ö	LYS	38	17.770	8.140	28.343 28.068	1.00	49.53
20	279	N	TRP	39	16.719	6.166	26.599	1.00	49.53
30	280	CA	TRP	39	16.634	6.286	25.919	1.00	52.24
	281	CB	TRP	39	17.250	5.060	26.016	1.00	52.24
	282 283	CG	TRP	39	18.742	4.956	25.124	1.00	52.24
	284	CD2	TRP	39	19.701	5.542	25.598	1.00	52.24
35	285	CE2	TRP	39	20.985	5.189 6.338	23.972		52.24
33	286	CE3	TRP	39	19.601	4.288	26.966		52.24
	287	CD1	TRP	39	19.461	4.422	26.720		52.24
	288	NE1	TRP	39	20.809	5.601	24.961		52.24
	289	CZ2	TRP	39	22.158	6.750	23.339		52.24
40		CZ3	TRP	39	20.772 22.032	6.380	23.837	1.00	52.24
	291	CH2	TRP	39	15.194	6.450	26.090	1.00	49.53
	292	С	TRP	39		5.831	26.608	1.00	49.53
	293	0	TRP	39		7.283	25.079		52.82
	294	N	PHE	40 40		7.470	24.529		52.82
45	5 295	CA	PHE	40		8.894	24.79		55.71
	296	CB	PHE	40		9.229	26.25		55.71 55.71
	297	CG	PHE PHE	40	44000	9.497	27.00		55.71 55.71
	298	CD1	PHE	40		9.208	26.90		55.71
_	299	CD2	PHE	40		9.719	28.36		55.71
5		CE1	PHE	40		9.437	28.28		55.71
	301	CE2	PHE	40		9.691	29.01		
	302	CZ	PHE	4		7.159	23.02	· -	
	303	C	PHE	4		7.823	22.22	·-	
_	304	0 N	HIS	4	1 12.896	6.117	22.66		
3	5 305	CA	HIS	4	1 12.766	5.703	21.26		
	306	CB	HIS	4	1 12.801	4.176	21.18		
	307	CG	HIS	4	1 12.708	3.643	19.79		
	308	CD2			1 12.249		19.3 18.6		
	309	ND1		4	1 13.128		17.6		
•	50 310 311	CE1		4	12.931		17.9	• .	·
	311	NE2		4	11 12.397		20.8		·
	312	C	HIS		11 11.408		20.6 21.4		
	313	ŏ	HIS		41 10.387	5.917	۲.۱۹		'
	314	_							

	315	N	ASN	42 -	11.419	7.145	19.845	1.00	49.72
	316	CA	ASN	42	10.184	7.785	19.375	1.00	49.72
	317	CB	ASN	42	9.253	6.782	18.668	1.00	43.66
	318	CG	ASN	42	9.743	6.393	17.280	1.00	43.66
5	319	OD1	ASN	42	10.632	7.053	16.729	1.00	43.66
	320	ND2	ASN	42	9.156	5.340	16.708	1.00	43.66
	321	С	ASN	42	9.447	8.391	20.562 20.609	1.00 1.00	49.72 49.72
	322	0	ASN	42	8.220	8.372 8.901	20.609 21.5 3 3	1.00	60.04
	323	N	GLY	43	10.202 9.588	9.505	22.706	1.00	60.04
10	324	CA	GLY GLY	43 43	9.566 9.100	8.539	23.778	1.00	60.04
	325	CO	GLY	43 43	8.465	8.961	24.748	1.00	60.04
	326 327	Ň	SER	44	9.377	7.247	23.615	1.00	55.75
	328	CA	SER	44	8.948	6.249	24.592	1.00	55.75
15	329	CB	SER	44	8.280	5.058	23.908	1.00	71.51
13	330	ÖĞ	SER	44	6.988	5.397	23.456	1.00	71.51
	331	Č	SER	44	10.118	5.744	25.405	1.00	55.75
	332	0	SER	44	11.122	5.289	24.855	1.00	55.75
	333	N	LEU	45	9.981	5.821	26.723	1.00	58.69
20	334	CA	LEU	45	11.040	5.380	27.609 29.068	1.00	58.69
	335	CB	LEU	45	10.639	5. 58 5	30.129	1.00 1.00	58.46 58.46
	336	CG	LEU	45	11.647	5.140 5.90 6	30.005	1.00	58.46
	337	CD1	LEU	45 45	12.963 11.017	5.358	31.491	1.00	58.46
25	338	CD2	LEU LEU	45 45	11.375	3.925	27.366	1.00	58.69
25	339 340	CO	LEU	45 45	10.508	3.054	27.398	1.00	58.69
	341	N	SER	46	12.650	3.677	27.116	1.00	59.18
	342	ĊA	SER	46	13.138	2.336	26.864	1.00	59.18
	343	CB	SER	46	14.437	2.402	26.077	1.00	54.40
30	344	OG	SER	46	15.025	1.120	26.000	1.00	54.40
	345	С	SER	46	13.388	1.591	28.165	1.00	59.18
	346	0	SER	46	13.461	2.192	29.236	1.00	59.18 69.21
	347	N	GLU	47	13.507	0.274	28.073 29.252	1.00 1.00	69.21
	348	CA	GLU	47	13.785	-0.524 -1. 944	29. 2 52 29. 0 80	1.00	88.33
35	349	CB	GLU GLU	47 47	13.256 11.752	-2.050	29.190	1.00	88.33
	350	CG CD	GLU	47	11.284	-3.483	29.278	1.00	88.33
	351 352	OE1	GLU	47	11.349	-4.198	28.256	1.00	88.33
	353	OE2	GLU	47	10.860	-3.898	30.377	1.00	88.33
40	354	Č	GLU	47	15.297	-0.541	29.433	1.00	69.21
	355	Ö	GLU	47	15.807	-0.973	30. 46 2	1.00	69.21
	356	N	GLU	48	16.003	-0.057	28.415	1.00	63.82
	357	CA	GLU	48	17.456	0.011	28.433	1.00	63.82
	358	CB	GLU	48	17.980	0.306	27.025	1.00	75.50 75.50
45	359	CG	GLU	48	19.483	0.478	26. 95 0 27. 46 6	1.00 1.00	75.50 75.50
	360	CD	GLU	48	20.223	-0.738 -1.802	27.400 26.810	1.00	75.50 75.50
	361	OE1	GLU	48 48	20.152 20.863	-0. 62 8	28.534	1.00	75.50
	362	OE2	GLU GLU	46 48	17.902	1.113	29.394	1.00	63.82
50	363 364	C O	GLU	48	17.454	2.255	29.284	1.00	63.82
50	365	Ň	THR	49	18.792	0.772	30.322	1.00	72.39
	366	ČA	THR	49	19.275	1.737	31.303	1.00	72.39
	367	CB	THR	49	18.867	1.316	32.727	1.00	60.69
	368	OG1	THR	49	19.140	-0.079	32.907	1.00	60.69
55	369	CG2	THR	49	17.381	1.573	32.953	1.00	60.69
	370	С	THR	49	20.780	2.007	31.294	1.00	72.39
	371	0	THR	49	21.247	2.896	31.998	1.00	72.39 68.99
	372	N	ASN	50	21.543	1.251	30.509	1.00	68.99
<i>_</i>	373	CA	ASN	50 50	22.991	1.473 0.247	30.445 29. 87 9	1.00 1.00	96.77
60		CB	ASN ASN	50 50	23.710 23.508	-0.989	30.733	1.00	96.77
	375 376	CG OD1	ASN	50 50	23.625	-0.933	31.956	1.00	96.77
	376	ND2	ASN	50	23.209	-2.114	30.092	1.00	96.77
	377 378	C	ASN	50	23.294	2.693	29.579	1.00	68.99
	5,5	_							

	379 380 381	O N CA	ASN SER SER	51 51	22.424 24.527 24.927	3.178 3.186 4.369 4.843	29.655	1.00 1.00 1.00 1.00	68.99 51.99 51.99 64.53
_	382	CB	SER SER		26.304 27.281	3.878	28.998	1.00	64.53
5	383 384	OG C	SER	51	24.978	4.074	27.391 26.569	1.00 1.00	51.99 51.99
	385	0	SER	51	25.024 24.998	4.987 2.793	27.045	1.00	68.17
	386	N	SER SER	52 52	25.600	2.395	25.650	1.00	68.17
10	387	CA CB	SER	52	26.351	1.690	25.346 25.123	1.00 1.00	64.58 64.58
10	388 389	OG	SER	52	27.361	2.655 1.502	25.123 25.248	1.00	68.17
	390	Ç	SER	52 52	23.866 23.621	0.468	25.864	1.00	68.17
	391	O N	SER LEU	52 53	23.136	1.927	24.221	1.00 1.00	42.59 42.59
15	392 393	CA	LEU	53	22.001	1.160 2.108	23.704 23.328	1.00	56.84
15	394	CB	LEU	53	20.856 19.581	1.569	22.678	1.00	56.84
	395	CG	LEU LEU	53 53	19.134	0.285	23.349	1.00	56.84 56.84
	396	CD1 CD2	LEU	53	18.501	2.627	22.801 22.473	1.00 1.00	42.59
20	397 398	C	LEU	53	22.434	0.407 1.009	21.545	1.00	42.59
20	399	0	LEU	53 54	23.049 22.330	-0.911	22.479	1.00	55.75
	400	N	ASN ASN	54 54	22.762	-1.722	21.349	1.00	55.75 73.05
	401 402	CA CB	ASN	54	23.530	-2.950	21.820 22.300	1.00 1.00	73.05
25	402	CG	ASN	54	24.921	-2.613 -2.024	21.565	1.00	73.05
20	404	OD1	ASN	54 54	25.717 25. 22 5	-2.984	23.539	1.00	73.05
	405	ND2	ASN ASN	54	21.592	-2.177	20.493	1.00	55.75 55.75
	406 407	C O	ASN	54	20.643	-2.806 1.835	20.979 19.212	1.00 1.00	67.23
30	408	Ň	ILE	55	21.660 20.623	-1.835 -2.237	18.281	1.00	67.23
,	409	CA	ILE	55 55	20.023	-1.098	17.338	1.00	49.71
	410	CB CG2	ILE ILE	5 5	19.390	-1.625	16.199	1.00 1.00	49.71 49.71
	411 412	CG1	ILE	5 5	19.512	-0.026 1.189	18.124 17.333	1.00	49.71
35	413	CD1	ILE	55 55	19.172 21.209	-3.398	17.498	1.00	67.23
	414	Ç	ILE ILE	55 55	22.197	-3.231	16.776	1.00	67.23 59.54
	415 · 416	0 N	VAL	56	20.618	-4.576	17.674 16.993	1.00 1.00	59.54
	417	CA	VAL	56	21.101 21.340	-5.774 -6.907	18.013	1.00	69.51
40) 418	CB	VAL	56 56	21.949	-8.114	17.311	1.00	69.51
	419	CG1 CG2	VAL VAL	56	22.262	-6.419	19.125	1.00 1.00	69.51 59.54
	420 421	C	VAL	56	20.152	-6.270 -6.289	15.898 16.086		59.54
	422	0	VAL	56	18.932 20.716	-6.20 3 -6.684	14.763	1.00	58.29
4	5 423	N	ASN ASN	57 57	19.932	-7.171	13.618		58.29 80.36
	424	CA CB	ASN	57	19.399	-8.588	13. 86 9 13. 9 01		80.36
	425 426	CG	ASN	57	20.503	-9.631 -9.723	12.977		80.36
	427	OD1	ASN	57 57	21.319 20.534	-10.428	14.966	1.00	80.36
5	0 428	ND2	ASN ASN	57		-6.195	13.433		58.29 58.29
	429 430	C O	ASN	57	17.619	-6.517	13.660 13.027		46.57
	431	N	ALA	58		-4.991 -3.885	12.84		46.57
	432	CA	ALA ALA	58 58		-2.774	12.07	5 1.00	27.34 46.57
	55 433	CB C	ALA	58	16.915	-4,227	12.17		46.57 46.57
	434 435	ŏ	ALA	58		-4.920 -3.732	11.14 12.73		53.79
	436	N	LYS	59 59			12.14	6 1.00	53.79
	437	CA	LYS	59 59		-4.514	13.16		70.29 70.29
•	60 438 439	CB CG	LYS	59	14.035	-5.733	13.91 15.11		70.29
	440	CD	LYS	59			16.03		70.29
	441	CE	LYS	59 59			17.18		70.29
	442	NZ	LYS	5					

	440	C	LYS	59 -	14.033	-2.579	11.682	1.00 1.00	53.79 53.79
	143 144	ŏ	LYS	59	14.593	-1.549	12.062 10.839	1.00	57.14
	144 445	Ň	PHE	60	13.011	-2.563	10.359	1.00	57.14
	446 446	CA	PHE	60	12.473	-1.301	9,355	1.00	75.29
	44 7	СВ	PHE	60	11.350	-1.5 49 -2.022	8.019	1.00	75.29
	44 8	CG	PHE	60	11.823	-2.022 -2.876	7.259	1.00	75.29
	449	CD1	PHE	60	11.028	-1.596	7.499	1.00	75.29
	450	CD2	PHE	60	13.043 11.437	-3.304	5.999	1.00	75.29
	451	CE1	PHE	60	13.465	-2.016	6.237	1.00	75.29
10	452	CE2	PHE	60 60	12.657	-2.873	5.485	1.00	75.29
	453	CZ	PHE	60	11.922	-0.568	11.567	1.00	57.14
	454	C	PHE	60	11.895	0.659	11.609	1.00	57.14
	455	0	PHE GLU	61	11.484	-1. 34 5	12.550	1.00	62.19
	456	N	GLU	61	10.921	-0.803	13.778	1.00	62.19 93.34
15	457	CA CB	GLU	61	10.401	-1.937	14.671	1.00 1.00	93.34
	458	CG	GLU	61	9.199	-2.699	14.121	1.00	93.34
	459 460	CD	GLU	61	9.496	-3.449	12.827 12.815	1.00	93.34
	460 461	OE1	GLU	61	10.425	-4.285 0.003	11.823	1.00	93.34
20	462	OE2	GLU	61	8.792	-3,203 0.013	14.552	1.00	62.19
20	463	C	GLU	61	11.960	0.932	15.285	1.00	62.19
	464	Ó	GLU	61	11.609 13.235	-0.315	14.384	1.00	48.05
	465	N	ASP	62	14.272	0.406	15.107	1.00	48.05
	466	CA	ASP	62	15.573	-0.389	15.119	1.00	36.56
25	467	CB	ASP	62 62	15.420	-1.725	15.809	1.00	36.56
	468	CG	ASP	62	14.696	-1.799	16.822	1.00	36.56
	469	OD1	ASP ASP	62	16.025	-2.703	15.355	1.00	36.56
	470	OD2	ASP	62	14.516	1.790	14.535	1.00	48.05 48.05
	471	C O	ASP	62	15.250	2.587	15.110	1.00 1.00	39.66
30	472	N	SER	63	13.896	2.076	13.399	1.00	39.66
	473 474	CA	SER	63	14.076	3.386	12.809 11.428	1.00	51.20
	47 4 475	CB	SER	63	13.420	3.454	10.524	1.00	51.20
	476	og .	SER	63	14.091	2.604 4.361	13.759	1.00	39.66
35	477	C	SER	63	13.419	3.966	14.630	1.00	39.66
55	478	Ο.	SER	63	12. 64 7 13. 72 2	5.637	13.613	1.00	35.00
	479	N	GLY	64 64	13.108	6.589	14.521	1.00	35.00
	480	CA	GLY	64	14.014	7.568	15.260	1.00	35.00
	481	C	GLY GLY	64	15.207	7.696	14.975	1.00	35.00
40		0	GLU	65	13.406	8.261	16.214	1.00	46.87 46.87
	483	N CA	GLU	65	14.075	9.259	17.020		64.86
	484	CB	GLU	65	13.101	10.390	17.340		64.86
	485 486	CG	GLU	65	13.685	11.460	18.222 18.727		64.86
45		CD	GLU	65		12.430	19.574		64.86
72	488	OE1	GLU	65		12.030 13.596	18.274	1.00	64.86
	489	OE2	GLU	65		8.683	18.327		46.87
	490	С	GLU	65		7.988	19.046	3 1.00	46.87
	491	0	GLU	65 66		8.985	18.632		50.39
50		N.	TYR	66		8.533	19.88		50.39 40.76
	493	CA	TYR TYR	66		7.535	19.60		40.76 40.76
	494	CB CG	TYR	6		6.188	19.14		40.76
	495 406	CD1	TYR	6	6 17.117	5.843	17.80		40.76
5	496 5 497	CE1	TYR	6	6 16.746	4.585	17.38 20.05		40.76
3	498	CD2		6		5.236	19.64		40.76
	499	CE2	TYR	6		3.973	18.31		40.76
	500	CZ	TYR	6			17.91		40.76
	501	OH	TYR		6 16.024		20.65		50.39
6	50 502	C	TYR		66 17.032 66 17.732		20.07		50.39
•	503	0	TYR				21.95	55 1.00	55.49
	504	N	LYS		67 16.719 67 17. 22 1		22.8		55.49
	505	CA	LYS LYS		37 16.106	44.500	23.3	79 1.00	68.70
	506	CB	LIO	`	- -				

									•
		CC	LYS	67 ·	15.118	12.362	22.412	1.00	68.70
	507	CG	LYS	67	13.879	12.767	23.199	1.00	68.70
	508	CD	LYS	67	12.818	13.407	22.338	1.00	68.70
	509	CE		67	11.597	13.688	23.149	1.00	68.70
-	510	NZ	LYS		17. 73 4	10.114	24.092	1.00	55.49
5	511	C	LYS	67 67		9.054	24.446	1.00	55.49
	512	0	LYS	67	17.209	10.658	24.759	1.00	60.89
	513	N	CYS	68	18.749		25.992	1.00	60.89
	514	CA	CYS	68	19.179	10.011	27.145	1.00	60.89
	515	С	CYS	68	19.028	10.988		1.00	60.89
10	516	0	CYS	68	18.795	12.193	26.946	1.00	
	517	CB	CYS	68	20.594	9.418	25.897		63.38
	518	SG	CYS	68	22.069	10.482	25.959	1.00	63.38
	519	N	GLN	69	19.113	10.457	28.355	1.00	61.40
	520	CA	GLN	69	18. 94 3	11.268	29.546	1.00	61.40
15	521	CB	GLN	69	17. 49 5	11.161	29.998	1.00	108.41
	522	CG	GLN	69	17.207	11.587	31.426	1.00	108.41
	523	CD	GLN	69	16.245	12.754	31.486	1.00	108.41
	524	OE1	GLN	69	15.641	13.126	30. 493	1.00	108.41
	525	NE2	GLN	69	16.097	13.333	32.665	1.00	108.41
20	526	C	GLN	69	19.858	10.792	30.642	1.00	61.40
20	527	ŏ	GLN	69	19.859	9.609	31.005	1.00	61.40
	528	Ň	HIS	70	20.653	11.729	31.139	1.00	103.97
	529	ČA	HIS	70	21.594	11.480	32.217	1.00	103.97
	530	CB	HIS	70	23.011	11.824	31.761	1.00	140.89
25		CG	HIS	70	24.032	11.697	32.844	1.00	140.89
23	531	CD2	HIS	70	24.744	12.638	33.503	1.00	140.89
	532	ND1	HIS	70	24.407	10.485	33.376	1.00	140.89
	533	CE1	HIS	70	25.311	10.685	34.319	1.00	140.89
	534	NE2	HIS	70	25.534	11.984	34.416	1.00	140.89
20	535		HIS	70 70	21,186	12.373	33.396	1.00	103.97
30	536	C	HIS	70	20.184	13.088	33.319	1.00	103.97
	537	0	GLN	71	21.968	12.364	34.470	1.00	101.70
	538	N		71	21.646	13.163	35.640	1.00	101.70
	539	CA	GLN	71	22.512	12.706	36.820	1.00	136.43
	540	CB	GLN	71	21.739	11.968	37.924	1.00	136.43
35	541	CG	GLN	71		11.194	38.876	1.00	136.43
	542	CD	GLN	71	22.639	11.696	39.322	1.00	136.43
	543	OE1	GLN	71	23.660		39.206	1.00	136.43
	544	NE2	GLN	71	22.242	9. 966 14.663	35.407	1.00	101.70
	545	. C	GLN	71	21.782		36.361	1.00	101.70
40	546	0	GLN	71	21.838	15.441	34.137	1.00	141.76
	547	N	GLN	72	21.778	15.065	33.755	1.00	141.76
	548	CA	GLN	72	21.905	16.470		1.00	141.59
	549	CB	GLN	72	22.748	16.587	32.494	1.00	141.59
	550	CG	GLN	72	24.182	16.131	32.710		141.59
45	551	CD	GLN	72	25.045	16.307	31.482	1.00	141.59
	552	OE1	GLN	72	24.616	16.858	30.472	1.00	
	553	NE2	GLN	72	26.285	15.841	31.570	1.00	141.59
	554	C	GLN	72	20.578	17.187	33.541	1.00	141.76
	555	0	GLN	72	20.531	18.246	32.918	1.00	141.76
50	556	N	VAL	73	19. 509	16.598	34.067	1.00	141.76
-	557	.CA	VAL	73	18.150	17.144	33.996	1.00	141.76
	558	СВ	VAL	73	17.945	18.230	35.093	1.00	113.45
	559	CG1	VAL	73	16.471	18.593	35.215	1.00	113.45
	560	CG2	VAL	73	18.475	17.718	36.424	1.00	113.45
55	561	c	VAL	73	17.677	17.707	32. 644	1.00	141.76
33	562	ŏ	VAL	73	16.643	18.376	32.568	1.00	141.76
	563	Ň	ASN	74	18.433	17.441	31.583	1.00	110.03
	564	CA	ASN	74	18.056	17.906	30.249	1.00	110.03
	565	CB	ASN	74	18.782	19.208	29.880	1.00	123.79
60	566	CG ·	ASN	74	18.013	20.459	30.295	1.00	123.79
w	567	OD1	ASN	74	16.818	20.402	30.597	1.00	123.79
		ND2	ASN	74	18.698	21.598	30.291	1.00	123.79
	568 569		ASN	74	18.382	16.840	29.212	1.00	110.03
	569 570	CO	ASN	74	19.531	16.412	29.094	1.00	110.03
	570	U	MON	/+	13.001	, V+ 7 1 L	20.00		

	571	N	GLU	75 ·	17.367	16.416	28.460	1.00	64.12
	571 572	CA	GLU	75	17.552	15.399	27.433	1.00	64.12
	572 573	CB	GLU	75	16.190	14.961	26.882	1.00	93.37
	574 ·	CG	GLU	75	15.332	14.330	27.971	1.00	93.37
5	575	CD	GLU	75	13.963	13.868	27.511	1.00	93.37
3	576	OE1	GLU	75	13.583	14.146	26.355	1.00	93.37
	577	OE2	GLU	75	13.264	13.227	28.327	1.00	93.37
	578	C	GLU	75	18.454	15.910	26.319	1.00	64.12
	579	Ŏ	GLU	75	18.591	17.118	26.120	1.00	64.12
10	580	Ñ	SER	76	19.090	14.984	25.611	1.00	56.18
	581	CA	SER	76	19.980	15.362	24.518	1.00	56.18
	582	СВ	SER	76	20.944	14.217	24.188	1.00	74.86
	583	OG	SER	76	20.235	13.084	23.720	1.00	74.86
	584	С	SER	76	19.189	15.720	23.263	1.00	56.18
15	585	0	SER	76	17.968	15.559	23.199	1.00	56.18 67.41
	586	N	GLU	77	19.896	16.237	22.271	1.00 1.00	67.41
	587	CA	GLU	77	19.250	16.561	21.021 20.096	1.00	96.50
	588	CB	GLU	77 	20.205	17.326 18.734	20.563	1.00	96.50
	589	CG	GLU	77 77	20.530 19.281	19.545	20.859	1.00	96.50
20	590	CD	GLU	77 77	18.406	19.638	19.973	1.00	96.50
	591	OE1	GLU GLU	77 77	19.173	20.089	21.978	1.00	96.50
	592	OE2	GLU	77	18.903	15.205	20.416	1.00	67.41
	593	C	GLU	77	19.605	14.210	20.646	1.00	67.41
25	594	0	PRO	78	7.805	15.136	19.660	1.00	64.74
25	595 500	N CD	PRO	78	16.712	16.106	19.495	1.00	62.17
	596 597	CA	PRO	78	17.447	13.852	19.067	1.00	64.74
	597 598	CB	PRO	78	16.047	14.101	18.514	1.00	62.17
	599	CG	PRO	78	15.527	15.197	19.372	1.00	62.17
30	600	Č	PRO	78	18.421	13.473	17.959	1.00	64.74
50	601	ŏ	PRO	78	19.118	14.321	17.404	1.00	64.74
	602	Ň	VAL	79	18.469	12.183	17.670	1.00	45.82
	603	ĊA	VAL	79	19.274	11.638	16.593	1.00	45.82
	604	СВ	VAL	79	20.455	10.798	17.123	1.00	63.76
35	605	CG1	VAL	79	21.165	10.108	15.972	1.00	63.76
	606	CG2	VAL	79	21.437	11.702	17.841	1.00	63.76
	607	С	VAL	79	18.266	10.745	15.857	1.00	45.82 45.82
	608	0	VAL	79	17.396	10.128	16.485	1.00 1.00	52.05
	609	N	TYR	80	18.347	10.697	14.533 13.790	1.00	52.05 52.05
40	610	CA	TYR	80	17.396	9.886 10.760	12.810	1.00	70.93
	611	CB	TYR	80	16.612	11.787	13.520	1.00	70.93
	612	CG	TYR	80	15.767 16. 32 9	12.975	13.998	1.00	70.93
	613	CD1	TYR	80 80	15.573	13.882	14.744	1.00	70.93
45	614	CE1	TYR TYR	80	14.422	11.533	13.798	1.00	70.93
45	615	CD2	TYR	80	13.656	12.427	14.543	1.00	70.93
	616 617	CE2 CZ	TYR	80	14.237	13.598	15.017	1.00	70.93
	618	OH	TYR	80	13.493	14.459	15.798	1.00	70.93
	619	Ċ.	TYR	80	18.016	8.711	13.074	1.00	52.05
50	620	ŏ	TYR	80	18.975	8.859	12.320	1.00	52.05
50	621	N	LEU	81	17.464	7.532	13.332	1.00	46.77
	622	ĊA	LEU	81	17.960	6.319	12.702	1.00	46.77
	623	CB	LEU	81	18.213	5.249	13.767	1.00	49.82
	624	CG	LEU	81	19.042	4.032	13.338	1.00	49.82
55	625	CD1	LEU	81	20.515	4.427	13.231	1.00	49.82
	626	CD2	LEU	81	18.884	2.907	14.354	1.00	49.82 46.77
	627	С	LEU	81	16.935	5.811	11.659	1.00	46.77
	628	0	LEU	81	15.720	5.865 5.837	11.881	1.00	44.84
	629	N	GLU	82	17.434	5.337	10.523	1.00 1.00	44.84
60		CA	GLU	82	16.568	4.816	9.487 8.395	1.00	75.78
	631	CB	GLU	82	16.372	5.863 5.412	7.277	1.00	75.78
	632	ÇG	GLU	82	15.459	5.412 6.571	6.490	1.00	75.78
	633	CD	GLU	82	14.890	7.613	6.387	1.00	75.78
	634	OE1	GLU	82	15.573	1.013	0.007		,

	ea5	OE2	GLU	82 ·	13.764	6.437		.00	75.78
	635 cae	C	GLU	82	17.124	3.526		1.00	44.84 44.84
	636 637	ŏ	GLU	82	18.256	3.478		1.00	58.13
	638	Ň	VAL	83	16.308	2.482		1.00 1.00	58.13
5	639	CA	VAL.	83	16.715	1.177		1.00	48.46
5	640	CB	VAL	83	16.204	0.070	8.909	1.00	48.46
	641	CG1	VAL	83	16.693	-1.285		1.00	48.46
	642	CG2	VAL	83	16.668	0.369 0.919		1.00	58.13
	643	С	VAL	83	16.212	1.088		1.00	58.13
10	644	0	VAL	83	15.033 17.118	0.509		1.00	54.77
	645	N .	PHE	84	16.772	0.235		1.00	54.77
	646	CA	PHE	84 84	17.572	1.115	3.750	1.00	54.95
	647	СВ	PHE	84	17.424	2.584	3.986	1.00	54.95
	648	CG	PHE PHE	84	18.222	3.227	4.937	1.00	54.95
15	649	CD1 CD2	PHE	84	16.503	3.336	3.246	1.00	54.95
	650	CE1	PHE	84	18.111	4.600	5.143	1.00	54.95
	651 652	CE2	PHE	84	16.378	4.708	3.438	1.00	54.95 54.95
	652 653	CZ	PHE	84	17.185	5.349	4.388	1.00 1.00	54. 5 5
20	654	č	PHE	84	17.031	-1.194	4.305 4.980	1.00	54.77
20	655	Ö	PHE	84	17.743	-1.947	4.960 3.148	1.00	50.72
	656	Ň	SER	85	16.474	-1.527	2.519	1.00	50.72
	657	CA	SER	85	16.625	-2.831 -3.696	2.776	1.00	85.41
	658	CB	SER	85	15.392	-4.996	2.253	1.00	85.41
25	659	OG	SER	85	15.578	-2.509	1.031	1.00	50.72
	660	С	SER	85 85	16.737 15.741	-2.1 6 6	0.397	1.00	50.72
	661	0	SER	85 86	17.933	-2.595	0.470	1.00	46.74
	662	N	ASP ASP	86	18.122	-2.283	-0.939	1.00	46.74
	663	CA	ASP	86	18.070	-0.766	-1.139	1.00	57.20
30	664	CB CB	ASP	86	17.810	-0.345	-2.581	1.00	57.20
	665	OD1	ASP	86	18.547	-0.781	-3.500	1.00	57.20 57.00
	666 667	OD2	ASP	86	16.866	0.442	-2.795	1.00	57.20 46.74
	668	C	ASP	86	19.4 9 9	-2.821	-1.277	1.00 1.00	46.74
35	669	ŏ	ASP	86	20.166	-3.402	-0. 429 -2.505	1.00	48.74
23	670	Ň	TRP	87	19.936	-2.615	-2.905 -2.935	1.00	48.74
	671	CA	TRP	87	21.241	-3.073 -3. 36 6	-4,440	1.00	51.62
	672	CB	TRP	87	21.226	-3.300 -4.704	-4.804	1.00	51.62
	673	CG	TRP	87	20.649 19.258	-5.039	-4.934	1.00	51.62
40	674	CD2	TRP	87 87	19.256	-6.406	-5.285	1.00	51.62
	675	CE2	TRP	87 87	18.064	-4.316	-4.793	1.00	51.62
	676	CE3	TRP TRP	87	21.344	-5.846	-5.072	1.00	51.62
	677	CD1 NE1	TRP	87	20.479	-6.872	-5 .3 61	1.00	51.62
4.5	678	CZ2	TRP	87	17.966	-7.069	-5.500	1.00	51.62
45	679 680	CZ3	TRP	87	16.849	-4.974	-5.006	1.00	51.62 51.62
	681	CH2	TRP	87	16.813	-6.337	-5.357 -2.634	1.00 1.00	48.74
	682	Č	TRP	87	22.285	-2.011	-2.034	1.00	48.74
	683	Ö	TRP	87	23.440	-2.327	-2. 29 7	1.00	48.62
50		N	LEU	88	21.889	-0.752 0.361	-2.517	1.00	48.62
	685	CA	LEU	88	22.774	1.159	-3.775	1.00	41.58
	686	CB	LEU	88		0.628	-4.731	1.00	41.58
	687	CG	LEU	88 88		1.715	-5.724	1.00	41.58
	688	CD1	LEU LEU	. 88		0.208	-3.975	1.00	41.58
5:		CD2	LEU	88		1.290	-1.503	1.00	48.62
	690	C	LEU	88		1.448	-1.458	1.00	48.62
	691	N	LEU	89		1.895	-0.683	1.00	46.32
	692 693	CA	LEU	89	22.532	2.823	0.336		46.32 41.30
6	0 694	CB	LEU	89		2.098	1.671		41.30
U	695	ÇG	LEU	89	22.014	2.940	2.913 2.656		41.30
	696	CD1	LEU	89		3.782	4.113		41.30
	697	CD2		89			0.459		46.32
	698	С	LEU	89	9 23.636	3.603	5. 100		

	699 700 701	O N CA	LEU LEU LEU LEU	89 - 90 90	24.821 23.259 24.233 23.818	3.509 5.134 6.196 7.418	0.353 1 0.489 1 -0.318	1.00 1.00 1.00 1.00	46.32 43.08 43.08 46.82
5	702 703 704 705	CB CG CD1 CD2 C	LEU LEU LEU LEU	90 90 90 90	24.810 26.217 24.344 24.229	8.588 8.116 9.655 6.528	-0.656 -1.270 1.975	1.00 1.00 1.00 1.00	46.82 46.82 46.82 43.08 43.08
10	706 707 708 709 710	O N CA CB	LEU GLN GLN GLN	90 91 91 91	23.177 25.404 25.484 26.177	6.760 6.493 6.817 5.695 4.377	2.588	1.00 1.00 1.00 1.00 1.00	44.37 44.37 39.09 39.09
15	711 712 713 714	CG CD OE1 NE2	GLN GLN GLN GLN	91 91 91 91 91	25.435 26.190 27.337 25.535 26.261	3.286 2.992 2.678 8.121	5.468 5.162 6.433 4.136	1.00 1.00 1.00 1.00	39.09 39.09 39.09 44.37
20	715 716 717 718	C O N CA CB	GLN GLN ALA ALA ALA	91 92 92 92	27.172 * 25.860 26.534 25.618	8.390 8.948 10.217 11.365	3.357 5.091 5.309 4.952	1.00 1.00 1.00 1.00	44.37 44.40 44.40 35.90 44.40
25	719 720 721 722 723	C O N CA	ALA ALA SER SER	92 92 93 93	26.921 26.223 28.025 28.435	10.332 9.806 11.019 11.214	6.767 7.631 7.041 8.419 8.493	1.00 1.00 1.00 1.00 1.00	44.40 39.65 39.65 42.29
	724 725 726 727	CB OG C O	SER SER SER SER	93 93 93 93 94	29.821 29.947 27.373 27.048 26.801	11.866 12.998 12.092 11.939 13.006	7.649 9.062 10.239 8.291	1.00 1.00 1.00 1.00	42.29 39.65 39.65 49.05
30	728 729 730 731	N CA CB C	ALA ALA ALA ALA ALA	94 94 94 94	25.759 26.397 24.815 25.238	13.865 15.014 14.416 14.702	8.848 9.617 7.775 6.668	1.00 1.00 1.00 1.00	49.05 25.45 49.05 49.05
35	732 733 734 735 736	N CA CB CG	GLU GLU GLU GLU	95 95 95 95	23.542 22.598 21.200 21.107	14,563 15,115 14,552 13,088	8.099 7.126 7.355 6.999 7.345	1.00 1.00 1.00 1.00 1.00	54.30 54.30 64.16 64.16 64.16
40	737	CD OE1 OE2 C	GLU GLU GLU	95 95 95 95	19.770 19.563 18.926 22.594	12.488 11.286 13.218 16.636 17.332	7.063 7.899 7.253 6.405	1.00 1.00 1.00 1.00	64.16 64.16 54.30 54.30
45	741 742 743 744	O N CA CB	GLU VAL VAL	95 96 96 96 96	22.044 23.234 23.366 22.414 22.662	17.127 18.550 19.000 20.472	8.317 8.595 9.707 10.030	1.00 1.00 1.00 1.00	54.64 54.67 44.67
50	745 746 747) 748 749	CG1 CG2 C O N	VAL VAL VAL VAL VAL	96 96 96 97	20,957 24,800 25,161	18.784 18.787 18.494 19.306	9.274 9.049 10.194 8.134	1.00 1.00 1.00 1.00	44.67 54.64 54.64 48.96 48.96
5:	750 751 752	CA CB CG1 CG2	VAL VAL VAL VAL	97 97 97 97	27.866 29.339 27.628	19.592 19.209 19.450 17.773 21.078	8.365 7.133 7.407 6.764 8.619	1.00 1.00 1.00 1.00 1.00	46.14 46.14 46.14 48.96
	754 755 756 757	C O N CA	VAL VAL MET MET	97 97 98 98	26.654 28.148 28.479	21.934 21.385 22.770 22.920	7.956 9.560 9.866 11.329	1.00 1.00 1.00 1.00	48.96 48.67 48.67 88.16
6	758 759 760 761 762	CB CG SD CE C	MET MET MET MET MET	98 98 98 91 91	27.724 28.143 28.281	22.792 23.133 21.471 23.222	12.290 14.001 14.634 8.937	1.00 1.00	88.16 88.16 88.16 48.67

					151	8.603	1.00	48.67
	0	MET	98 - 30.	70.	22.451	8.488	1.00	51.28
763	N		99 29.		24.467	7.5 7 9	1.00	51.28
764			99 30		25.003		1.00	66.75
765	CA	GLU	99 30	.227	26.488	7.339	1.00	66.75
76 6	СВ	GLU		.195	27.175	6.403	1.00	66.75
5 767	CG	GLU		.842	28.632	6.164	1.00 1.00	66.75
768	CD	GLU	99 30	.515	29.334	7.146		66.75
769	OE1	GLU		.901	29.072	4.994	1.00	51.28
<i>7</i> 70	OE2	GLU		.939	24.801	8.133	1.00	51.28
771	C	GLU		2.182	25.000	9.318	1.00	56.63
10 772	0	GLY		2.874	24.401	7.280	1.00	56.63
7 73	N			4.233	24.185	7.748	1.00	56.63
<i>7</i> 74	CA	GLY GLY		4.534	22.752	8.172	1.00	56.63
<i>7</i> 75	Ç	GLY		5.670	22.300	8.074	1.00	64.74
<i>7</i> 76	0			3.519	22.037	8.654	1.00	64.74
15 777	N _.	GLN		3.683	20.645	9.065	1.00	
778	CA	GLN		2.550	20.236	10.003	1.00	77.71 77.71
<i>7</i> 79	СВ	GLN		2.559	20.959	11.325	1.00	
780	CG	GLN		3.844	20.719	12.090	1.00	77.71
781	CD	GLN		4.912	_1.200	11.702	1.00	77.71
20 782	OE1	GLN		33.751	19.957	13.179	1.00	77.71
783	NE2	GLN		33.695	19.702	7.855	1.00	64.74
784	С	GLN		33.327	20.083	6.745	1.00	64.74
785	0	GLN		34.132	18.452	8.055	1.00	53.53
786	N	PRO		34.809	17.877	9.236	1.00	44.31
25 787	CD	PRO		34.163	17.510	6.936	1.00	53.53
788	CA	PRO		35.317	16.590	7.311	1.00	44.31
789	CB	PRO		35.0 9 7	16.438	8.790	1.00	44.31
790	CG	PRO		32.841	16.752	6.795	1.00	53.53
791	С	PRO		32.064	16.635	7.739	1.00	53.53
30 792	0	PRO		32.604	16.242	5.596	1.00	42.44
793	N	LEU		31.403	15.480	5.300	1.00	42.44
794	CA	LEU	103	30.500	16.243	4.317	1.00	43.14
795	CB	LEU	103	29.332	15.406	3.768		43.14
796	CG	LEU	103	28.454	14.974	4.920		43.14
35 797	CD1	LEU	103	28.522	16.193	2.768	1.00	43.14
798	CD2	LEU	103	31.845	14.169	4.673	1.00	42.44
799	С	LEU	103	32.569	14.163	3.679	1.00	42.44
800	0	LEU	103	31.429	13.052	5.246	1.00	40.42
801	N	PHE	104	31.825	11.772	4.659		40.42
40 802		PHE	104	32.503	10.860	5.701		57.95
803	CB	PHE	104	33.631	11.515	6.453	3 1.00	57.95
804	CG	PHE	104	33.383	12.232	7.62		57.95
808	CD1	PHE	104	34.943	11.411	6.00	3 1.00	57.95
806		PHE	104	34.436	12.836	8.34	1 1.00	57.95
45 807	CE1	PHE	104	35.999	12.011	6.71	4 1.00	57.95
80	B CE2	PHE	104	35.741	12.721	7.88	0 1.00	57.95
80	g CZ	PHE	104	30.635	11.025	4.04	5 1.00	40.42
81	D C	PHE	104	29.571	10.908	4.66		40.42
81	1 0	PHE	104	30.837	10.528	2.83	3 1.00	44.12
50 81		LEU	105	29.810	9.765	2.14		44.12
81	3 CA	LEU	105	29.383	10.445	0.84		40.26
81		LEU	105	28.872	11.866	0.98		40.26
81	5 CG	LEU	105	28.555	12.435	-0.30	67 1.00	40.26
81	16 CD:		105	27.668	11.857	1.8	99 1.00	40.26
55 B1		2 LEU	105	30.382	8.393	1.8	29 1.00	44.12
	18 C	LEU	105	31.587		1.6	39 1.00	44.12
	19 0	LEU	105	29.497		1.7	45 1.00	
	20 N	ARG	106			1.4		45.34
	21 CA	ARG	106	29.912		2.8	29 1.00	57.54
	22 CB	ARG	106		1		1.00	57.54
, a	23 CG	ARG	106				62 1.00	57.54
	24 CD) ARG	106				356 1.00	57.54
	25 NE	ARG	106				297 1.00	
	26 CZ		106	30.501	1.6.6			
`								

		400	106 - 29.516	1.530	6.128 1.	.00	57.54
827	NH1	ARG	106 31.110	0.040		.00	57.54
828	NH2	ARG	106 28.800	5.359		.00	45.34
829	C	ARG ARG	106 27.658	5.345		.00	45.34
830	0	CYS	107 29.129	4.824		.00	48.19
5 831	N	CYS	107 28.156	4.098		.00	48.19
832	CA	CYS	107 28.337	2.663		.00	48.19
833	C O	CYS	107 29.268	1.948		.00	48.19
834	СВ	CYS	107 28.474	4.238		.00	54.03
835	SG	CYS	107 27.089	3.836		.00	54.03
10 836 837	N	HIS	108 27.430	2.286		.00	52.57 53.57
838	ČA	HIS	108 27.433	1.009		.00	52.57 42.83
839	CB	HIS	108 26.986	1.261		1.00 1.00	42.83
840	CG	HIS	108 27.086	0.067		1.00	42.83
15 841	CD2	HIS	108 26.211	-0.448		1.00	42.83
842	ND1	HIS	108 28.214	-0.725 -1.677	4.092	1.00	42.83
843	CE1	HIS	108 28.026	-1.531		1.00	42.83
844	NE2	HIS	108 26.820	-0.048		1.00	52.57
845	С	HIS	108 26.567 108 25.398	0.192		1.00	52.57
20 846	0	HIS		-1.226		1.00	46.92
847	N	GLY		-2.313		1.00	46.92
848	CA	GLY	109 26.413 109 25.824	-3.310		1.00	46.92
849	Č	GLY	109 26.406	-3.596		1.00	46.92
850	0	GLY TRP	110 24.657	-3.840	-0.063	1.00	39.32
25 851	N	TRP	110 23.983	-4.832		1.00	39.32
852	CA	TRP	110 22.807	-5.430		1.00	37.53
853	CB CG	TRP	110 22.002	-6.428		1.00	37.53
854	CD2	TRP	110 20.978	-6.153		1.00	37.53
855 30 856	CE2	TRP	110 20.507	-7.399	2.183	1.00	37.53
30 856 857	CE3	TRP	110 20.414	-4.973	2.225	1.00	37.53
858	CD1	TRP	110 22.105	-7.785	0.672	1.00	37.53 37.53
859	NE1	TRP	110 21.212	-8.376	1.531	1.00 1.00	37.53 37.53
860	CZ2	TRP	110 19.494	-7.508	3.152	1.00	37.53 37.53
35 861	CZ3	TRP	110 19.400	-5.078	3.195 3.645	1.00	37.53
862	CH2	TRP	110 18.954	-6.344	1,134	1.00	39.32
863	С	TRP	110 24.991	-5.918 -6.297	0.309	1.00	39.32
864	0	TRP	110 25.816	-6.405	2.369	1.00	45.97
865	N	ARG	111 24.938 111 25.876	-7.4 4 7	2.818	1.00	45.97
40 866	CA	ARG	111 25.876 111 25.607	-8.754	2.093	1.00	58.00
867	CB	ARG	111 24.357	-9.430	2.525	1.00	58.00
868	CG	ARG ARG	111 24.273	-10.832	1.934	1.00	58.00
869	CD	ARG	111 23.403	-11.623	2.786	1.00	58.00
870	NE CZ	ARG	111 23.773	-12.728	3.406	1.00	58.00
45 871 872	NH1	ARG	111 25.005	-13.203	3.260	1.00	58.00
873	NH2	ARG	111 22.918	-13.322	4.218	1.00	58.00 45.97
874	_	ARG	111 27.337	-7.099	2.583	1.00	45.97 45.97
875		ARG	111 28.184	-7.996	2.501	1.00	52.35
50 876		ASN	112 27.645	-5.817	2.438 2.172	1.00 1.00	52.35
877		ASN	112 29.017	-5.420 5.700	3.341	1.00	76.11
878		ASN	112 29.923	-5.796 -4.718	4.374	1.00	76.11
879	CG	ASN	112 29.974	-3.629	4.117	1.00	76.11
880		ASN	112 30.488	-3.02 <i>5</i> -4.997	5.553	1.00	76.11
55 881		ASN	112 29.427 112 29.581	-6.010	0.883	1.00	52.35
882		ASN	112 29.581 112 30.778	-6.304	0.792	1.00	52.35
883		ASN	113 28.719	-6.180	-0.110	1.00	53.59
884		TRP TRP	113 29.177	-6.682	-1.386	1.00	53.59
889		TRP	113 27.991	-6.922	-2.333	1.00	53.83
60 88		TRP	113 27.170		-1.993	1.00	53.83
88	•	TRP	113 25.778		-2.273	1.00	53.83
88 88		TRP	113 25.440	-9.634	-1.783	1.00	53.83
89		TRP	113 24.779		-2.895	1.00	53.83
09	J J_0	• • • •	•				

					07.007	-9.273	-1.368	1.00	53.83
	391	CD1	. ,	113 ·	27.607	-10.173	-1.236	1.00	53.83
		NE1	TRP	113	26.578	-10.173	-1.888	1.00	53.83
	892 892	CZ2	TRP	113	24.144	-10.105 -8.107	-3.002	1.00	53.83
	893	CZ3	TRP	113	23.490	-8.107 -9.394	-2.500	1.00	53.83
	894	CH2	TRP	113	23.186		-1.939	1.00	53.59
	895	C	TRP	113	30.068	-5.583	-1.605	1.00	53.59
	896	ŏ	TRP	113	29.892	-4.407	-1.003 -2.779	1.00	64.92
	897		ASP	114	31.022	-5.950	-3.363	1.00	64.92
	898	N	ASP	114	31.893	-4.950	-3.303 -4.020	1.00	80.11
	899	CA	ASP	114	33.105	-5.602		1.00	80.11
10	900	CB	ASP	114	33,906	-6.427	-3.046	1.00	80.11
	901	CG	ASP	114	34.241	-5.892	-1.968	1.00	80.11
	902	OD1	ASP	114	34.195	-7.603	-3.355	1.00	64.92
	903	OD2	ASP	114	31.122	-4.148	-4.390	1.00	64.92
	904	Ç	ASP	114	30.332	-4.691	-5.170	1.00	69.99
15	905	0	VAL	115	31.343	-2.844	-4.375		69.99
	906	N		115	30.680	-1.966	-5.309	1.00	39.79
	907	CA	VAL	115	29.938	-0.86 5	-4.556	1.00	39.79 39.79
	908	CB	VAL	115	29.177	0.018	-5.530	1.00	39.79
	909	CG1	VAL	115	28.996	-1.485	-3.555	1.00	69.99
20	910	CG2	VAL	115	31.764	-1.376	-6.198	1.00	69.99
	911	С	VAL	115	32.797	-0.930	-5.701	1.00	
	912	0	VAL		31.540	-1.392	-7.511	1.00	52.13
	913	N	TYR	116	32.524	-0.869	-8.457	1.00	52.13
	914	- CA	TYR	116	33.016	-1.988	-9.377	1.00	78.35
25	915	CB	TYR	116	33.716	-3.109	-8.650	11.00	78.35
	916	ÇG	TYR	116		-4.214	-8.178	1.00	78.35
	917	CD1	TYR	116		-5.247	-7.492	1.00	78.35
	918	CE1	TYR	116		-3.057	-8.419	1.00	78.35
	919	CD2	TYR	116		-4.077	-7.736	1.00	78.35
30	920	CE2	TYR	116		-5.170	-7.275	1.00	78.35
50	921	CZ	TYR	116		-6.180	-6.600	1.00	78.35
	922	OH	TYR	116		0.258	-9.292	1.00	52.13
	923	С	TYR	116		0.507	-9.242	1.00	52.13
	924	Ó	TYR	116		0.933	-10.063	1.00	52.62
35	925	N	LYS	117		2.040	-10.901	1.00	52.62
25	926	CA	LYS	117		1.523	-12.102	1.00	75.37
	927	СВ	LYS	11		0.848	-13.200		75.37
	928	CG	LYS	11			-14,444	1.00	75.37
	929	CD	LYS	11			-14.904	1.00	75.37
40		CE	LYS	11			-16.222	2 1.00	75.37
40	931	NZ	LYS	11			-10.099	5 1.00	52.62
	932	C	LYS	11			-10.58		52.62
	933	Ö	LYS	11		·	-8.85		53.28
	934	Ň	VAL	111			-8.02		53.28
45		CA	VAL	11			-6.56		39.37
4.	936	СВ	VAL	11	18 31.52		-5.79		39.37
	937	CG1	VAL		18 30.80		-5.90		39.37
	938	CG2	VAL		18 31.21		-8.51		53.28
	939	Č	VAL		18 31.04	- 400	-8.77		53.28
_		ŏ	VAL		18 32.10	- 0470	-8.66		50.90
5	941	Ň	ILE		19 29.84		-9.07		50.90
	_	C _A	ILE	1	19 29.70		-10.48		47.00
	942	ČВ	ILE	1	19 29.09		-10.8		47.00
	943	CG2		1	119 28.89		-10.5	-·	47.00
	944	CG1		1	119 30.02		-12.9		47.00
2	55 945	CD1	_	1	119 29.50	7.082	-12.9		50.90
	946		ILE		119 28.7				
	947	C	ILE		119 27.7				
	948	0	TYR		120 29.0	87 9.429			
	949	N	TYR		120 28.2	28 10.172		·	· •
(60 950	CA	TYR		120 29.0	18 10.751			4
	951	CB			120 29.5	₁₀₈ 9.727			
	952	CG			120 30.7	64 9.150			
	953	CD			120 31.2) -3.6	342 1.00	, 71.11
	954	CE	1 TYR	,					

						9.332	-3.518	1.00	47.71
	955	CD2	TYR	120 -	28.716	8.376		1.00	47.71
	956	CE2	TYR	120	29.167 30.427	7.820	-2.781	1.00	47.71
	957	CZ	TYR	120 120	30.894	6.859	-1.911	1.00	47.71
	958	OH	TYR	120	27.559	11.319	-7.483	1.00	46.78
5	959	C	TYR TYR	120	28.166	11.972	-8.330	1.00	46.78 39.53
	960	0	TYR	121	26.306	11.572	-7.152	1.00	39.53 39.53
	961	N CA	TYR	121	25.578	12.651	-7.807 0.594	1.00 1.00	51.28
	962	CB	TYR	121	24.378	12.092	-8.584 0.758	1.00	51.28
10	963 964	CG	TYR	121	24.767	11.242	-9.758 -9.598	1.00	51.28
10	965	CD1	TYR	121	25.075	9.897	-10.673	1.00	51.28
	966	CE1	TYR	121	25.525	9.131 11.802	-11.025	1.00	51.28
	967	CD2	TYR	121	24.909	11.046	-12.106	1.00	51.28
	968	CE2	TYR	121	25. 35 9 25.669	9.712	-11.920	1.00	51.28
15	969	CZ	TYR	121 121	26.158	8.978	-12.979	1.00	51.28
	970	OH	TYR TYR	121	25.079	13.703	-6.834	1.00	39.53
	971	C	TYR	121	24.692	13.392	-5.711	1.00	39.53 48.43
	972	0	LYS	122	25.104	14.955	-7.2 63	1.00	48.43
00	973	N CA	LYS	122	24.584	16.022	-6.422	1.00 1.00	57.69
20	974 975	CB	LYS	122	25. 704	16.886	-5.851 -4.630	1.00	57.69
	975 976	CG	LYS	122	25.215	17.619	-4.345	1.00	57.69
	977	CD	LYS	122	25.990	18.882 19.987	-5.251	1.00	57.69
	978	CE	LYS	122	25.543	21.258	-4.865	1.00	57.69
25	979	NZ	LYS	122	26.178 23. 65 8	16.871	-7.296	1.00	48.43
	980	С	LYS	122 122	24.108	17.523	-8.231	1.00	48.43
	981	0	LYS	123	22.368	16.861	-6.983	1.00	47.40
	982	N.	ASP ASP	123	21.384	17.609	-7.783	1.00	47.40 40.57
	983	CA	ASP	123	21.625	19.122	-7.687	1.00	49.57 49.57
30	984	CB CB	ASP	123	21.713	19.611	-6.269	1.00 1.00	49.57
	985	OD1	ASP	123	20.803	19.311	-5. 468	1.00	49.57
	986 987	OD1	ASP	123	22.699	20.301	-5.9 5 3 -9.241	1.00	47.40
	988	C	ASP	123		17.197	-10.095	1.00	47.40
35	989	ŏ	ASP	123		18.044 15.904	-9.521	1.00	52.66
55	990	N	GLY	124		15.430	-10,888	1.00	52.66
	991	CA	GLY	124		15.363	-11.421	1.00	52.66
	992	С	GLY	124 124		14.382	-12.041	1.00	52.66
	993	0	GLY	12:		16.408	-11.204	1.00	53.89
40		N	GLU GLU	12		16.447	-11.672	1.00	53.89
	995	CA CB	GLU	12		17.841	-11.427	1.00	115.76 115.76
	996	CG	GLU	12	5 25.113	18.952	-12.208		115.76
	997 998	CD	GLU	12	5 25.418	18.876	-13.689 -14.044		115.76
45		OE1	GLU	12		18.910	-14.498		115.76
٦.	1000	OE2	GLU	12		18.784 15.412	-10.974		53.89
	1001	С	GLU	12		15.130	-9.790		53.89
	1002	0	GLU	12		14.847	-11.709	1.00	51.23
	1003	N	ALA	12 12		13.880	-11.125	1.00	51.23
5	0 1004	CA	ALA		26 28.557	12.996	-12.218		49.62
	1005	CB	ALA ALA		26 29.05	14.673	-10.422		51.23 51.23
	1006	C	ALA		26 29.659	15.551	-11.020		63.08
	1007	Ň	LEU		27 29.302	14.373	-9.15		63.08
5	1008 5 1009	CA	LEU		27 30.332	15.088	-8.40 ⁵ -7.10		50.82
2	1010	CB	LEU	1:	27 30.641	14.370	-7.10 -6.00		50.82
	1011	CG	LEU		27 29.663		-4.68		50.82
	1012	CD1	LEU		27 30.265		-6.00		50.82
	1013	CD2	LEU		27 29.403 27 31.643		-9.14	2 1.00	63.08
(50 1014	Ç	LEU				-9.68	8 1.00	63.08
	1015	0	LEU		27 32.233 28 32.096	4	-9.13	1.00	120.62
	1016	N	LYS		128 33.343		-9.78		120.62
	1017	CA CB	LYS LYS		28 33.360		-10.12	20 1.00	105.58
	1018	ÇB	LIO						

	1019 1020 1021	CG CD CE	LYS LYS LYS	128 128 128 128	32.187 32.494 31.295 30.167	18.879 20.181 20.661 21.011	-10.946 -11.667 -12.465 -11.563	1.00 1.00 1.00	105.58 105.58 105.58 105.58
5	1022 1023 1024	NZ C O N	LYS LYS LYS TYR	128 128 128 129	34.535 35.604 34.353	16.589 16.232 16.714	-8.883 -9.381 -7.568	1.00 1.00 1.00 1.00	120.62 120.62 102.50 102.50
	1025 1026 1027 1028	CA CB CG	TYR TYR TYR	129 129 129	35.415 34.823 34.316 32.980	16.387 16.167 17.406 17.523	-6.613 -5.216 -4.528 -4.148	1.00 1.00 1.00	91.38 91.38 91.38
10	1029 1030 1031	CD1 CE1 CD2	TYR TYR TYR TYR	129 129 129 129	32.519 35.187 34.741	18.664 18.455 19.598	-3.477 -4.224 -3.557	1.00 1.00 1.00	91.38 91.38 91.38 91.38
15	1032 1033 1034 1035	CE2 CZ OH C	TYR TYR TYR	129 129 129	33.408 32.960 36.133	19.699 20.831 15.099 14.244	-3.185 -2.533 -7.024 -7.692	1.00 1.00 1.00 1.00	91.38 102.50 102.50
20	1036 1037 1038	O N CA CB	TYR TRP TRP TRP	129 130 130 130	35.553 37.394 38.102 39.605	14.948 13.709 13.916	-6.636 -6.940 -7.127	1.00 1.00 1.00 1.00	95.53 95.53 77.30 77.30
	1039 1040 1041 1042	CB CG CD2 CE2	TRP TRP TRP	130 130 130	40.317 40.414 41.001 40.046	12.599 11.594 10.447 11.536	-7.015 -8.027 -7.440 -9.379	1.00 1.00 1.00	77.30 77.30 77.30
25	1043 1044 1045	CE3 CD1 NE1 CZ2	TRP TRP TRP TRP	130 130 130 130	40.853 41.262 41.229	12.046 10.752 9.269	-5.881 -6.124 -8.149	1.00 1.00 1.00 1.00	77.30 77.30 77.30 77.30
30	1046 1047 1048 1049	CZ3 CH2 C	TRP TRP TRP	130 130 130	40.278 40.862 37.903 38.038	10.365 9.250 12.742 13.124	-10.083 -9.469 -5.784 -4.620	1.00 1.00 1. 0 0	77.30 95.53 95.53
25	1050 1051 1052	O N CA CB	TRP TYR TYR TYR	130 131 131 131	37.589 37.397	11.488 10.505 10.495	-6.091 -5.034 -4.565	1.00 1.00 1.00 1.00	71.08 71.08 66.47 66.47
35	1053 1054 1055 1056	CG CD1 CE1	TYR TYR TYR	131 131 131	34.894 34.370 33.355	10.405 9.178 9.111 11.562	-5.657 -6.055 -7.009 -6.246	1.00 1.00 1.00	66.47 66.47 66.47
40	1057	CD2 CE2 CZ OH	TYR TYR TYR TYR	131 131 131 131	33.375 32.857 31.819	11.506 10.283 10.246 9.098	-7.201 -7.572 -8.477 -5.384	1.00	66.47 66.47 66.47 71.08
45	1061 1062 1063	C 0 N	TYR TYR GLU GLU	13 ¹ 13 13 13	1 38.058 2 37.970	8.768 8.277 6.884	-6.554 -4.345 -4.467	1.00 1.00 1.00	71.08 130.21 130.21 141.76
	1064 1065 1066 1067	CA CB CG CD	GLU GLU	13 13 13	2 39.252 2 38.484 2 39.311	6.520 6.649 7.221 7.379	-3.266 -1.959 -0.824 -0.989	1.00 1 1.00	141.76 141.76 141.76
50	1068 1069 1070	OE1 OE2 C	GLU GLU GLU	13 13 13 13	32 38.717 32 37.135	7.507 6.013 6.503	0.239 -4.479 -4.23	9 1.00 9 1.00 4 1.00	141.76 130.21 130.21 122.18
5	1071 1072 5 1073 1074	O N CA CB	ASN ASN ASN	13 13 13	33 37.307 33 36.182 33 36.698 33 35.592	3.803	-4.74 -4.79 -5.09 -5.50	4 1.00 0 1.00 2 1.00	122.18 141.76 141.76
6	1075 1076 1077 50 1078	CG OD1 ND2 C	ASN	1: 1 1	33 34.412 33 35.986 33 35.346	1.777 0 0.200 8 3.806	-5.52 -5.83 -3.50 -2.40	1 1.00 5 1.00	122.18
	1079 1080 1081 1082	O N CA CB	ASN HIS HIS HIS	1	33 35.87 34 34.04 34 33.01 34 32.50	4 4.032 3 4.052	-3.68 -2.63 -2.3!	31 1.00 30 1.00	110.94

	1083	CG	HIS	134 -	33.300	1.858	-1.341	1.00	116.53
	1084	CD2	HIS	134	33.153	1.742	-0.001	1.00	116.53
	1085	ND1	HIS	134	34.341	1.029	-1.687	1.00	116.53
	1086	CE1	HIS	134	34.797	0.425	-0.605	1.00	116.53
5	1087	NE2	HIS	134	34.091	0.837	0.431	1.00	116.53
•	1088	C	HIS	134	33.169	4.773	-1.283	1.00	110.94
	1089	Ö	HIS	134	32.312	4.627	-0.408	1.00	110.94
	1090	Ň	ASN	135	34.245	5.532	-1.105	1.00	107.95
	1091	CA	ASN	135	34.430	6.296	0.125	1.00	107.95
10	1092	CB	ASN	135	35.464	5.654	1.057	1.00	141.21
10	1093	ČĞ	ASN	135	35.389	6.207	2.490	1.00	141.21
	1094	OD1	ASN	135	34.536	7.044	2.801	1.00	141.21
	1095	ND2	ASN	135	36.271	5.735	3.358	1.00	141.21
	1096	C	ASN	135	34.900	7.680	-0.310	1.00	107.95
15	1097	ŏ	ASN	135	35.952	7.836	-0.925	1.00	107.95
15	1098	Ň	ILE	136	34.095	8.685	-0.005	1.00	65.75
	1099	CA	ILE	136	34.421	10.048	-0.387	1.00	65.75
	1100	СВ	ILE	136	33.401	10.550	-1.433	1.00	6 5.18
	1101	CG2	ILE	136	32.002	306	-0.943	1.00	65.18
20	1102	CG1	ILE	136	33.587	12.030	-1.717	1.00	65.18
20	1103	CD1	ILE	136	32.601	12.535	-2.780	1.00	65.18
	1104	Č.	ILE	136	34.457	10.983	0.826	1.00	65.75
	1105	ŏ	ILE	136	33.593	10.924	1.706	1.00	65.75
	1106	N	SER	137	35.475	11.838	0.863	1.00	51.67
25	1107	CA	SER	137	35.646	12.785	1.957	1.00	51.67
23	1107	CB	SER	137	36.944	12.470	2.714	1.00	87.54
	1109	OG	SER	137	37.068	13.249	3.889	1.00	87.54
	1110	C	SER	137	35.678	14.225	1.449	1.00	51.67
	1111	ŏ	SER	137	36.522	14.593	0.629	1.00	51.67
30	1112	Ň	ILE	138	34.729	15.021	1.924	1.00	63.18
50	1113	ČA	ILE	138	34.634	16.431	1.559	1.00	63.18
	1114	CB	ILE	138	33.178	16.801	1.239	1.00	64.58
	1115	CG2	iLE	138	33.030	18.301	1.103	1.00	64.58
	1116	CG1	ILE	138	32.754	16.080	-0.043	1.00	64.58
35	1117	CD1	ILE	138	31.285	16.134	-0,328	1.00	64.58
33	1118	C.	ILE	138	35.119	17.126	2.815	1.00	63.18
	1119	ŏ	ILE	138	34.379	17.271	3.786	1.00	63.18
	1120	Ň	THR	139	36.384	17.525	2.783	1.00	80.92
	1121	CA	THR	139	37.063	18.140	3.920	1.00	80.92
40	1122	CB	THR	139	38.557	18.282	3.609	1.00	76.51
40	1123	OG1	THR	139	38.721	19.040	2.403	1.00	76.51
	1124	CG2	THR	139	39.189	16.909	3.432	1.00	76.51
	1125	C	THR	139	36.576	19.468	4.498	1.00	80.92
	1126	ŏ	THR	139	36.484	19.612	5.721	1.00	80.92
45	1127	Ň	ASN	140	36.277	20.441	3.644	1.00	57.80
43	1128	CA	ASN	140	35.837	21.738	4.151	1.00	57.80
	1129	СВ	ASN	140	36.840	22.821	3.731	1.00	95.08
	1130	ČĠ	ASN	140	37.066	23.863	4.812	1.00	95.08
	1131	OD1	ASN	140	36.122	24.315	5.458	1.00	95.08
50	1132	ND2	ASN	140	38.320	24.259	5.005	1.00	95.08
50	1133	C	ASN	140	34.438	22.108	3.657	1.00	57.80
	1134	ŏ	ASN	140	34.300	22.924	2.752	1.00	57.80
	1135	Ň	ALA	141	33.413	21.512	4.265	1.00	63.45
	1136	CA	ALA	141	32.031	21.765	3.871	1.00	63.45
55	1137	CB	ALA	141	31.060	21.206	4.914	1.00	40.09
20	1138	Č	ALA	141	31.740	23.242	3.642	1.00	63.45
	1139	ŏ	ALA	141	32.185	24.106	4.399	1.00	63.45
	1140	N	THR	142	30.971	23.505	2.588	1.00	60.40
	1141	CA	THR	142	30.573	24.847	2.192	1.00	60.40
60		CB	THR	142	31.247	25.210	0.871	1.00	65.36
50	1143	0G1	THR	142	32.580	25.646	1.137	1.00	65.36
	1144	CG2	THR	142	30,489	26.292	0.144	1.00	65.36
	1145	č	THR	142	29.062	24.871	2.017	1.00	60.40
	1146	ŏ	THR	142		23.815	1.955	1.00	60.40
	. 1-10	•			÷ · · · · 				

				4.49	28.471	26.061			51.83
11	47	N	VAL	143 ·	27.031	26.150		1.00	51.83
11	48	CA	VAL	143	26.547	27.626	1.744	1.00	51.35
	49	CB	VAL	143	27.058	28.335	0.507	1.00	51.35
11	50	CG1	VAL VAL	143	25.019	27.673	1.807	1.00	51.35
	151	CG2	VAL	143	26.667	25.448	0.434	1.00	51.83
	152	C	VAL	143	25.584	24.884	0.292	1.00	51.83 54.88
11	153	O N	GLU	144	27.599	25.466	-0.513	1.00 1.00	54.88
11	154	CA	GLU	144	27.411	24.836	-1.812	1.00	66.83
10 4	155 456	CB	GLU	144	28.554	25.200	-2.749 -3.146	1.00	66.83
	156 157	CG	GLU	144	28.639	26.639	-3.1 40 -3.860	1.00	66.83
	157 158	CD	GLU	144	29.941	26.929	-3.300 -4.799	1.00	66.83
	159	OE1	GLU	144	30.280	26.169	-3.478	1.00	66.83
	160	OE2	GLU	144	30.624	27. 90 8 23.308	-1.754	1.00	54.88
15 1	161	С	GLU	144	27.348	22.675	-2.685	1.00	54.88
	162	0	GLU	144	26.862 27.869	22.707	-0.692	1.00	47.71
	163	N	ASP	145	27.840 27.840	21.258	-0.607	1.00	47.71
	1164	CA	ASP	145	28.902	20.746	0.360	1.00	46.72
	1165	CB	ASP	145 145	30.292	21.045	-0.116	1.00	46.72
	1166	CG	ASP ASP	145	30.613	20.700	-1.268	1.00	46.72
	1167	OD1	ASP	145	31.077	21.629	0.667	1.00	46.72
	1168	OD2	ASP	145	26.463	20.785	-0.200	1.00	47.71
	1169	C	ASP	145	26.227	19.592	-0.055	1.00	47.71 42.81
	1170	0 N	SER	146	25.549	21.727	-0.007	1.00	42.81
	1171	CA	SER	146	24.175	21.355	0.314	1.00 1.00	49.76
	1172	CB	SER	146	23.363	22.573	0.750	1.00	49.76
	1173	OG	SER	146	23.841	23.139	1.955 -0.993	1.00	42.81
	1174 1175	Č	SER	146	23.583	20.794	-0.993 -2.091	1.00	42.81
30	1176	ŏ	SER	146	24.014	21.160 19.905	-0.879	1.00	56.97
30	1177	N	GLY	147		19.334	-2.064	1.00	56.97
	1178	CA	GLY	147		17.975	-1.766	1.00	56.97
	1179	С	GLY	147		17.546	-0.612	1.00	56.97
	1180	0	GLY	147		17.294	-2.797	1.00	35.67
35	1181	N	THR	148 148		15,968	-2.594	1.00	35.67
	1182	CA	THR	148		15.784	-3.251	1.00	41.21
	1183	CB	THR THR	148		15.127	-4.522	1.00	41.21
	1184	OG1	THR	148		17.118	-3.427	1.00	41.21 35.67
40	1185	CG2	THR	148		15.106	-3.297	1.00	35.67 35.67
40	1186	C O	THR	14	3 21.853	15.447	-4.382	1.00 1.00	37.71
	1187 1188	N	TYR	149	9 21.743	13.998	-2.668 -3.233	1.00	37.71
	1189	CA	TYR	14		13.118	-3.233 -2.317	1.00	40.71
	1190	CB	TYR	14		13.045	-2.117		40.71
45	1191	CG	TYR	14	9 24.803	14.300 15.396	-1.442		40.71
7.5	1192	CD1	TYR	14		16.544	-1.214		40.71
	1193	CE1	TYR	14		14.366	-2.568		46.71
	1194	CD2	TYR	14		15.494	-2.357		40.71
	1195	CE2	TYR	14	·	16.581	-1.680		40.71
50	1196	CZ	TYR TYR	14		17.712	-1.50€		40.71
	1197	ŎН	TYR		9 22.234	11.701	-3.349		37.71
	1198	CO	TYR		49 21.256	11.316	-2.690		37.71 32.88
	1199	N	TYR		50 22.918	10.930	-4.18		32.88
55	1200	CA	TYR		50 22.629		-4.33°		48.85
55	1201 1202	CB	TYR	1	50 21. 32 5		-5.12		48.85
	1202	CG	TYR		50 21.384		-6.60 -7.48		48.85
	1203	CD1	TYR		50 21.813		-7.40 -8.85		48.85
	1205	CE1	TYR		50 21.854		-0.63 -7.13		48.85
60		CD2	TYR		50 20.997		-8.50		48.85
	1207	CE2	TYR		50 21.038		-9.35		48.85
	1208	CZ	TYR		50 21.470 50 21.566		-10.70	00.1	48.85
	1209	ОН	TYR		150 21.566 150 23.85		-5.04		32.88
	1210	С	TYR		الماري الماري	3.550			

				04	000	9.802	-5.513	1.00	32.88
	1211	0	TYR		.668	7.699	-5.108	1.00	43.72
	1212	N	CYS		.018		-5.793	1.00	43.72
	1213	CA	CYS		.173	7.151	-6.660	1.00	43.72
	1214	Č.	CYS		.734	5.984		1.00	43.72
5		ŏ	CYS		.634	5.457	-6.488	1.00	45.51
3	1215	СВ	CYS	151 26	.229	6.672	-4.779		45.51
	1216	SG	CYS	151 25	.716	5.340	-3.631	1.00	49.22
	1217		THR	152 25	.605	5.601	-7.588	1.00	
	1218	N	THR		5.366	4.470	-8.467	1.00	49.22
	1219	CA	THR		5.033	4.892	-9.940	1.00	42.84
10	1220	CB	THR		3.153	5.566	-10.535	1.00	42.84
	1221	OG1			3.823	5.794	-9.968	1.00	42.84
	1222	CG2	THR		6.647	3.655	-8.467	1.00	49.22
	1223	Ç	THR		7.752	4.192	-8.290	1.00	49.22
	1224	0	THR		6.501	2.352	-8.638	1.00	49.54
15	1225	N .	GLY		7.664	1.499	-8.669	1.00	49.54
	1226	CA	GLY		7.298	0.134	-9.203	1.00	49.54
	1227	С	GLY		6.118	-0.243	-9.243	1.00	49.54
	1228	0	GLY		8.314	-0.610	-9.618	1.00	50.10
	1229	N	LYS		8.108	-1.946	-10.141	1.00	50.10
20	1230	CA	LYS		9.078	-2.209	-11.297	1.00	64.36
	1231	CB	LYS	,		-3.599	-11.885	1.00	64.36
	1232	CG	LYS		8.956	-3.925	-12.851	1.00	64.36
	1233	CD	LYS		30.078	-5.382	-13.286	1.00	64.36
	1234	CE	LYS		30.006	-5.728	-14.324	1.00	64.36
25	1235	NZ	LYS		31.019	-5.726 -2.994	-9.048	1.00	50.10
23	1236	С	LYS		28.310	-2. 954 -3.123	-8.497	1.00	50.10
	1237	Ō	LYS		29.402		-8.714	1.00	62.56
	1238	N	VAL		27.236	-3.709	-7.727	1.00	62.56
	1239	CA	VAL		27. 29 5	-4.784 -4.722	-6.732	1.00	41.01
30	1240	CB	VAL		26.139	-5.872	-5.742	1.00	41.01
-	1241	CG1	VAL		26.266	-3.391	-6.009	1.00	41.01
	1242	CG2	VAL		26.132	-6.063	-8.546	1.00	62.56
	1243	С	VAL	,	27.163	-6.224	-9.312	1.00	62.56
	1244	0	VAL		26.211	-6.975	-8.380	1.00	74.40
35	1245	N	TRP	•	28.110	-8.205	-9,159	1.00	74.40
•	1246	CA	TRP		28.104 26.846	-9.049	-8.887	1.00	64.29
	1247	CB	TRP	156	26.728	-9.536	-7.464	1.00	64.29
	1248	CG	TRP	156 456	27.569	-10.497	-6.808	1.00	64.29
	1249	CD2	TRP	156 456	27.114	-10.605	-5.472	1.00	64.29
40	1250	CE2	TRP	156	28.661	-11.276	-7.218	1.00	64.29
	1251	CE3	TRP	156	25.826	-9.119	-6.528	1.00	64.29
	1252	CD1	TRP	156 156	26.052	-9.753	-5.330	1.00	64.29
	1253	NE1	TRP	156	27.717	-11.464	-4.537	1.00	64.29
	1254	CZ2	TRP	156	29.260	-12.130	-6.290	1.00	64.29
45	1255	CZ3	TRP	156	28.783	-12.215	-4.961	1.00	64.29
	1256	CH2	TRP	156	28.162	-7.814	-10.639	1.00	74.40
	1257	Ç	TRP		29.121	-7.178	-11.088	1.00	74.40
	1258	0	TRP	156 157	27.128	-8.163	-11.397	1.00	71.89
	1259	N	GLN	157	27.132	-7.841	-12.823	1.00	71.89
50) 1260	CA	GLN	157	26.876	-9.105	-13.650		111.42
	1261	CB	GLN	157	28.041	-10.072	-13.672		111.42
	1262	ÇĢ	GLN	157	29.351	-9.380	-13.965		111.42
	1263	CD	GLN	157	29.504	-8.683	-14.969		111.42
	1264	OE1	GLN	157	30.312	-9.570	-13.08	1 1.00	111.42
5	5 1265	NE2	GLN	157	26.192	-6.731	-13.29		71.89
	1266	Ç	GLN	157	26.153	-6.418	-14.47		71.89
	1267	0	GLN		25.437	-6.124	-12.38		61.40
	1268	N	LEU	158 158	24.522	-5.061	-12.78	9 1.00	61.40
	1269	CA	LEU	158	23.078	-5.463	-12.46	9 1.00	60.41
6	0 1270	CB ·	LEU	158	22.575	-6.756	-13.11	3 1.00	60.41
	1271	CG	LEU	158	21.104	-6.948	-12.77	7 1.00	60.41
	1272	CD1		158	22.778	-6.677	-14.60	5 1.00	60.41
	1273	CD2	LEU	158	24.822	-3.703	-12.14	1.00	61.40
	1274	С	LEU	150					

	4075	0	LEU	158 ·	25.619	-3.596	-11. 21 3 -12.662	1.00 1.00	61.40 56.42
	1275	Ň	ASP	159	24.167	-2.668	-12.140	1.00	56.42
	1276 1277	CA .	ASP	159	24.338	-1.322 -0.311	-13.276	1.00	74.24
	1278	CB	ASP	159	24.465	-0.586	-14.170	1.00	74.24
	1279	CG	ASP	159	25.653	-0.666	-13,663	1.00	74.24
	1280	OD1	ASP	159	26.7 9 4 25.444	-0.721	-15.392	1.00	74.24
	1281	OD2	ASP	159	23.135	-6.972	-11.282	1.00	56.42
	1282	С	ASP	159 159	21.992	-1.211	-11.680	1.00	56.42
	1283	0	ASP	160	23.390	-0.419	-10.098	1.00	43.45
10	1284	N	TYR TYR	160	22.303	-0.038	-9.214	1.00	43.45 50.12
	1285	CA	TYR	160	22.309	-0.884	-7.936	1.00 1.00	50.12
	1286	CB CG	TYR	160	22.158	-2.369	-8.182 -8.705	1.00	50.12
	1287	CD1	TYR	160	23.210	-3.115	-8.933	1.00	50.12
15	1288 1289	CE1	TYR	160	23.076	-4.483 -3.026	-7.896	1.00	50.12
13	1290	CD2	TYR	160	20.961	-4.392	-8.121	1.00	50.12
	1291	CE2	TYR	160	20.814 21.875	-5.113	-8.637	1.00	50.12
	1292	CZ	TYR	160 160	21.760	-6.467	-8.840	1.00	50.12
	1293	OH	TYR	160	22.384	1.437	-8.868	1.00	43.45
20	1294	C	TYR TYR	160	23.341	2.125	-9.219	1.00	43.45 46.75
	1295	0	GLU	161	21.370	1.922	-8.175	1.00 1.00	46.75
	1296	N CA	GLU	161	21.304	3.318	-7.810	1.00	65.60
	1297	CB	GLU	161	20.454	4.057	-8.847 -8.439	1.00	65.60
25	1298 1299	CG	GLU	161	19.930	5.421 6.190	-9.614	1.00	65.60
23	1300	CD	GLU	161	19.318	7.226	-9.377	1.00	65.60
	1301	OE1	GLU	161	18.653 19.517	5.765	-10.777	1.00	65.60
	1302	OE2	GLU	161		3.385	·-6.4 3 2	1.00	46.75
	1303	Ç	GLU GLU	161 161		2.702	-6.148	1.00	46.75
30	1304	0	SER	162		4.190	-5.559	1.00 1.00	41.55 41.55
	1305	N CA	SER	162		4.297	-4.202 -3.241	1.00	41.77
	1306	CB	SER	162	21.841	4.761	-3.467	1.00	41.77
	1307 1308	OG	SER	162		6.124 5.311	-4.170	1.00	41.55
35	1309	č	SER	162		6.079	-5.103	1.00	41.55
33	1310	0	SER	162		5.294	-3.088	1.00	45.18
	1311	N	GLU	16: 16:		6.261	-2.881	1.00	45.18
	1312	CA	GLU GLU	16	•	5.907	-1.632		80.94 80.94
	1313	CB	GLU	16		4.687	-1.787		80.94
40		CG CD	GLU	16		4.941	-2.730		80.94
	1315	OE1	GLU	16	3 14.163	5.812	-2.407 -3. 7 94		80.94
	1316 1317	OE2	GLU	16		4.285 7.576	-3.75° -2.653		45.18
	1318	Č_	GLU	16		7.576 7.581	-2.23		45.18
45		0	GLU	16		8.709	-2.92	3 1.00	47.28
	1320	N	PRO	16	64 16.592	8.936	-3.57	1.00	31.71
	1321	CD	PRO PRO		64 18.598	9.970	-2.71		47.28 31.71
	1322	CA	PRO		64 17.888	10.913	-3.67		31.71
	1323	CB CG	PRO		64 16.472	10.450	-3.55 -1.25		47.28
5	0 1324 1325	Č	PRO		64 18.525	10.444	-0.49		47.28
	1326	ŏ	PRO		64 17.624	10.084 11.263	-0.86		31.92
	1327	N	LEU		65 19.480	11.769	0.49		31.92
	1328	CA	LEU		65 19.513 65 20.705	44.400	1.22	8 1.00	52.60
5	5 1329	CB	LEU		65 21.098		2.56		52.60
	1330	CG	LEU LEU		165 19.980		3.50		52.60
	1331	CD1			165 22.404	11.139	3.0		
	1332	CD2 C	LEU		165 19.697	13.275	0.44 -0.4		
- 4	1333 50 1334	ŏ	LEU		165 20.401		-0. 4 1.3		
•	1335		ASN		166 19.084		1.3		38.25
	1336	CA	ASN		166 19.297 166 17.969		1.5	43 1.00	38.79
	1337	CB	ASN		166 17.969 166 17.059		0.3	09 1.00	38.79
	1338	CG	ASN		130 ,1130	-			

į

1	339 340	OD1 ND2	ASN ASN ASN	166 166 166	17.546 15.748 20.341	15.847 16.259 15.889	-0.801 0.490 2.398	1.00 1.00 1.00	38.79 38.79 38.25
	341	C .	ASN	166	20.282	15.480	3.561	1.00 1.00	38.25 41.84
	1342 1343	N	ILE	167	21.309	16.695	1.978 2.894	1.00	41.84
_	1344	CA	ILE	167	22.326 23.732	17.187 16.672	2.516	1.00	52.89
	1345	CB	ILE	167 167	24.814	17.546	3.159	1.00	52.89
	1346	CG2	ILE ILE	167	23.884	15.227	2.997	1.00	52.89 52.89
	1347	CG1 CD1	ILE	167	25.008	14.493	2.326 2.934	1.00 1.00	41.84
	1348 1349	Č.	ILE	167	22.356	18.698 19.347	1.905	1.00	41.84
	1350	0	ILE	167	22.535 22.194	19.250	4.132	1.00	49.92
	1351	N	THR THR	168 168	22.134	20.694	4.336	1.00	49.92
	1352	CA CB	THR	168	20.999	21.151	5.122	1.00 1.00	52.27 52.27
15	1353 1354	OG1	THR	168	19.818	20.706	4.465 5.238	1.00	52.27
	1355	CG2	THR	168	20.977	22.658 21.157	5.126	1.00	49.92
	1356	С	THR	168	23.434 23.768	20.577	6.156	1.00	49.92
	1357	0	THR VAL	168 169	24.078	22.216	4.649	1.00	52.96
20	1358	N CA	VAL	169	25.230	22.791	5.331	1.00	52.96 44.29
	1359 1360	CB	VAL	169	26.359	23.106	4.346 5.112	1.00 1.00	44.29
	1361	CG1	VAL	169	27.578	23.646 21.865	3.560	1.00	44.29
	1362	CG2	VAL	169	26.710 24.837	24.102	6.037	1.00	52.96
25	1363	C	VAL VAL	169 169	24.456	25.058	5.373	1.00	52.96 50.65
	1364	0 N	ILE	170	24.920	24.138	7.372	1.00 1.00	52.65 52.65
	1365 1366	CA	ILE	170	24.585	25.345	8.146 9.380	1.00	54.27
	1367	CB	ILE	170	23.700	25.033 24.342	8.945	1.00	54.27
30	1368	CG2	ILE	170 170	22.411 24.473	24.181	10.390	1.00	54.27
	1369	CG1	ILE ILE	170	23.644	23.798	11.619	1.00	54.27 52.65
	1370	CD1 C	ILE	170	25.841	26.060	8.638	1.00 1.00	52.65 52.65
	1371 1372	ŏ	ILE	170		25.488	8.620 9.075	1.00	92.13
35	1373	Ň	LYS	171	25.697	27.308 28.070	9.551	1.00	92.13
-	1374	CA	LYS	171 171		29.574	9.470	1.00	112.78
	1375	CB CB	LYS LYS	171		30.436	9.745	1.00 1.00	112.78 112.78
	1376 1377	CD	LYS	171	27.599	31.881	9.293 7. 77 2	1.00	112.78
40	1378	CE	LYS	171		32.008 33.430	7.772	1.00	112.78
	1379	NZ	LYS	171 171		27.674	10.974	1.00	92.13
	1380	C	LYS LYS	17		27.384	11.812		92.13 124.64
	1381 1382	0 N	ALA	173	28.551	27.662	11.230		124.64
45		CA	ALA	17		27.282 27.553	12.529 12.537		104.18
43	1384	CB	AĹA	17:		27.933 27.910	13.772	1.00	124.64
	1385	C	ALA ALA	17 17		27.191	14.695	1.00	124.64 141.76
	1386	0 N	PRO	17		29.254	13.819		113.27
50	1387) 1388	CD	PRO	17	3 28.819	30.230	12.825 14.963		141.76
50	1389	CA	PRO	17		29.953 31.354	14.41		113.27
	1390	CB	P30	17 17		31.556	13.57	5 1.00	113.27
	1391	CG	PRO PRO		73 26.461	29.332	15.55		141.76 141.76
5:	1392 5 1393	C O	PRO		73 25.733		14.87 16.82		135.93
J.	1394	Ň	ARG		74 26.219		17.59		135.93
	1395	CA	ARG		74 25.070 74 24.358	-	18.25	6 1.00	141.76
	1396	CB	ARG		74 24.358 74 25.304		19.06	5 1.00	141.76
,	1397	CG CD	ARG ARG		74 24.573	32.197	19.96		141.76 141.76
6	0 1398 1399	NE	ARG	1	74 25.519	32.986	20.75 21.74		141.76
	1400	CZ	ARG		74 25.17		22.07		141.76
	1401	NH1			74 23.90° 74 26.11	•	22.40		141.76
	1402	NH2	2 ARG	'		-			

					04.000	28.322	16.796	1.00	135.93
	1403	С	ARG	• • •	24.068	27.095	16.923	1.00	135.93
	1404	Ö	ARG	174	24.026	-8.090	14.864	1.00	113.42
	1405	C1	NAG	21A	25.553 26.103	-8.923	13.694	1.00	113.42
	1406	C2	NAG	21A	25.455	-8.533	12.455	1.00	113.42
5	1407	N2	NAG	21A	26.186	-8.153	11.409	1.00	113.42
•	1408	C7	NAG	21A	27.417	-8.115	11.428	1.00	113.42
	1409	07	NAG	21A	25,436	-7.756	10.148	1.00	113.42
	1410	C8	NAG	21A	25.876	-10.419	13.955	1.00	113.42
	1411	СЗ	NAG	21A 21A	26.513	-11.185	12.940	1.00	113.42
10	1412	O3	NAG	21A	26.441	-10.817	15.323	1.00	113.42
	1413	C4	NAG	21A	26.084	-12.164	15.616	1.00	113.42
	1414	04	NAG	21A	25.905	-9.887	16.423	1.00	113.42
	1415	C5	NAG NAG	21A	26.175	-8.502	16.092	1.00	113.42 113.42
	1416	O5	NAG	21A	26.569	-10.164	17,760	1.00	113.42
15	1417	C6	NAG	21A	26.198	-9.199	18.732	1.00	74.70
	1418	06	NAG	42A	9.440	5.012	15.315	1.00	74.70 74.70
	1419	C1	NAG	42A	8.867	3.648	14.939	1.00	74.70
	1420	C2	NAG	42A	9.316	2.609	15.844	1.00 1.00	74.70
43.4%	1421	N2 C7	NAG	42A	8.618	2.342	16.941	1.00	74.70
20	1422	07	NAG	42A	7.605	2.973	17.251	1.00	74.70
	1423	C8	NAG	42A	9.129	1.223	17.840	1.00	74.70
	1424	C3	NAG	42A	9.294	3.312	13.516	1.00	74.70
	1425	03	NAG	42A	8.752	2.058	13.131 12.538	1.00	74.70
25	1426	C4	NAG	42A	8.835	4.399	11.266	1.00	74.70
25	1427 1428	04	NAG	42A	9.469	4.168	13.046	1.00	74.70
	1429	C5	NAG	42A	9.262	5.795	14.433	1.00	74.70
	1430	O5	NAG	42A	8.894	6.001	12.259	1.00	74.70
	1431	C6	NAG	42A		6.900 7.808	11.744	1.00	74.70
30	1432	06	NAG	42A		3.603	10.203	1.00	81.02
30	1433	C1	NAG	42B		3.832	8.945	1.00	81.02
	1434	C2	NAG	42B		5.248	8.651	1.00	81.02
	1435	N2	NAG	428		5.828	8.641	1.00	81.02
	1436	C7	NAG	425	10.935 11.980	5.214	8.866	1.00	81.02
35	1437	07	NAG	42E		7.317	8.327	1.00	81.02
-	1438	C8	NAG	42E		3.068	7. 75 0	1.00	81.02
	1439	C3	NAG	42E 42E		3.298	6.616	1.00	81.02
	1440	О3	NAG	421	-	1.604	8.138		81.02
	1441	C4	NAG	42		0.730	7.000		81.02 81.02
4(04	NAG	42		1.393	9.341		81.02
	1443	C5	NAG NAG	42		2.187	10.472		81.02
	1444	O5	NAG	42		-0.057	9.812		81.02
	1445	C6	NAG	42		-0.235	10.916		121.66
	1446	O6 C1	MAN	42		0.362	6.612		121.66
4	5 1447	C2	MAN	42	C 7.465	0.370	5.06		121.66
	1448	O2	MAN	42	C 8.504	1.176	4.523 4.48		121.66
	1449	C3	MAN	42	C 7.571	-1.048	4.40		121.66
	1450 1451	03	MAN	42	C 8.850	-1.599	5.04		
5	0 1452	C4	MAN		C 6.480	-1.965	4.27		
د	1453	04	MAN		2C 5.296	-1.845	6.51		
	1454	C5	MAN		2C 6.167		7.12	_	
	1455	O 5	MAN		2C 7.300		7.33	•	121.66
	1456	C6	MAN		2C 5.858		6.52	-	121.
4	55 1457	O6	MAN		2C 5.372		-0.65		69.14
•	1458	C1	NAG		66A 14.879		-0.27		69.14
	1459	C2	NAG		66A 13.401	44.050	0.26		69.14
	1460	N2	NAG		66A 13.208		1.50	65 1.00	69.14
	1461	C7	NAG			•	2.3		69.14
	60 1462	07	NAG				2.0	65 1.0	
	1463	C8	NAG				-1.5		
	1464		NAG		166A 12.51: 166A 11.13		-1.1		
	1465				166A 12.83		-2.2	09 1.0	0 69.14
	1466	; C4	NAG		,				

1.

•	1467 1468 1469	O4 C5 O5	NAG NAG NAG NAG	166A 1	2.124 4.346 5.072 4.736	17.873 17.962 17.789 19.321	-2.463 -1.224 -3.074	1.00 1.00 1.00	69.14 69.14 69.14 69.14 69.14
5	1470 1471 1472 1473	C6 O6 C1 C2	NAG NAG NAG	166B 1	15.449 11.515 11.108 12.288	20.162 19.084 19.132 19.054	-2.169 -3.754 -5.235 -6.081	1.00 1.00 1.00 1.00	88.70 88.70 88.70
10	1474 1475 1476 1477	N2 C7 O7 C8	NAG NAG NAG	166B 166B 166B	12.566 11.857 13.816 10.337	17.929 16.927 17.904 20.432	-6.736 -6.667 -7.601 -5.516	1.00 1.00 1.00 1.00	88.70 88.70 88.70 88.70
15	1478 1479 1480 1481	C3 O3 C4 O4	NAG NAG NAG NAG	166B 166B 166B	9.844 9.165 8.572	20.426 20.603 21.908 20.469	-6.848 -4.535 -4.731 -3.089	1.00 1.00 1.00 1.00	88.70 88.70 88.70 88.70
13	1482 1483 1484 1485	C5 O5 ^^ O6	NAG NAG NAG NAG	166B 166B 166B 166B	9.688 10.358 8.612 9.186	19.203 20.538 20.529 22.047	-2.919 -2.021 -0.721 -4.475	1.00 1.00 1.00 1.00	88.70 88.70 88.70 140.23
20	1486 1487 1488	C1 C2 O2 C3	MAN MAN MAN MAN	166C 166C 166C 166C	7.210 6.971 8.186 6.384	23.248 23.629 24.444	-3.529 -2.897 -4.292	1.00 1.00 1.00 1.00	140.23 140.23 140.23 140.23
25	1489 1490 1491 1492	O3 C4 O4	MAN MAN MAN MAN	166C 166C 166C 166C	7.294 5.054 4.019 5.141	24.880 24.047 24.073 22.640	-5.294 -4.942 -3.966 -5.572	1.00 1.00 1.00	140.23 140.23 140.23 140.23
30	1493 1494 1495 1496	C5 O5 C6 O6	MAN MAN MAN	166C 166C 166C 1000	6.527 4.497 3.935 17.505	22.236 22.590 21.313 20.612	-5.734 -6.946 -7.207 -1.007	1.00 1.00 1.00 1.00	140.23 140.23 68.91
	1497 1498 1499 1500	OH2 OH2 OH2 OH2	WAT WAT WAT	1001 1002 1003	8.876 24.042 18.824	15.888 8.073 3.262 -6.784	-2.154 7.063 -1.304 -6.997	1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91
35	1501 1502 1503 1504	OH2 OH2 OH2 OH2	WAT WAT WAT WAT	1004 1005 1006 1007	20.414	-7.978 -8.042 5.554	-9. 80 1 14.310 -0.296 12.004	1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91
40	1505 1506 1507	OH2 OH2 OH2	WAT WAT WAT	1008 1009 1010 1011	15.148 20.894	2.758 17.603 14.371 -2.803	2.679 -7.289 0.523	1.00 1.00 1.00	68.91 68.91 68.91 68.91
45	1508 1509 1510 1511	OH2 OH2 OH2 OH2	WAT WAT WAT	1012 1013 1014 1015	2 23.414 3 15.450 4 20.819	-6.190 4.228 19.173 -12.922	4.824 29.002 25.674 -8.874	1.00 1.00 1.00	68.91 68.91 68.91
	1512 1513 1514 1515	OH2 OH2 OH2 OH2	TAW TAW TAW	101 101 101	6 20.297 7 12.264 8 10.662	0.066 10.290 12.690 28.860	-4.940 21.606 26.479 10.139	1.00	68.91 68.91 68.91 68.91
50		OH2 OH2 OH2 OH2	WAT WAT WAT WAT	101 102 102 102	0 10.314 1 29.439 2 35.124	0.397 18.571 0.026	3.316 -2.750 -10.50 8.31	6 1.00 6 1.00 B 1.00	68.91 68.91 68.91 68.91
5	1520 5 1521 1522	OH2 OH2 OH2 OH2		102 102 102 102	24 29.558 25 28.174	1.088	9.23 -11.72 0.70	6 1.00 6 1.00 9 1.00	68.91 68.91 68.91 68.91
ć	1523 1524 1525 50 1526 1527	OH2 OH2 OH2 OH2	TAW TAW TAW	10: 10: 10: 10	27 28.026 28 25.503 29 16.927 30 32.003	9.375 10.725 6.822	20.41 10.44 -7.39 32.04 21.29	5 1.00 6 1.00 17 1.00 94 1.00	68.91 68.91 68.91 68.91
	1528 1529 1530	OH2 OH2 OH2	WAT	10	31 12.466 32 15.327 33 11.530	0.065	19.12 33.99		68.91 68.91

	4504	OH2	WAT	1034 - 18.003	7.978	-6.726	1.00	68.91
	1531	OH2	WAT	1035 34.477	2.731	-7.719	1.00	68.91
	1532	OH2	WAT	1036 25.373	34.820	8.269	1.00	68.91
	1533	OH2	WAT	1037 14.026	16.389	25.301	1.00	68.91
5	1534 1535	OH2	WAT	1038 30.733	30.153	16.022	1.00	68.91
J	1536	OH2	WAT	1039 25.276	21.121	-10.191	1.00	68.91
	1537	OH2	WAT	1040 16.971	8.768	-11.221	1.00	68.91
	1538	OH2	WAT	1041 26.997	12.580	36.282	1.00	68.91
	1539	OH2	WAT	1042 5.954	6.575	17.557	1.00	68.91
10	1540	OH2	WAT	1043 26.429	-14.196	14.154	1.00	68.91
10	1541	OH2	WAT	1044 41.801	6.111	-5.021	1.00	68.91
	1542	OH2	WAT	1045 16.712	8.152	1.031	1.00	68.91
	1543	OH2	WAT	1046 10.222	17.172	0.994	1.00	68.91
	1544	OH2	WAT	1047 26.531	8.260	28.436	1.00	68.91
15	1545	OH2	WAT	1048 17.529	12.929	2.834	1.00	68.91
	1546	OH2	WAT	1049 31.571	12.227	-10.072	1.00	68.91
	1547	OH2	WAT	1050 22.536	1.995	35.016	1.00	68.91
	1548	OH2	WAT	1051 26.121	6.724	-12.642 2.327	1.00 1.00	68.91 68.91
	1549	OH2	WAT	1052 14.788	0.096	-8. 95 9	1.00	68.91
20	1550	OH2	WAT	1053 36.387	12.151 -9.146	-4.152	1.00	68.91
	1551	OH2	WAT	1054 30.213	21.863	-0.263	1.00	68.91
	1552	OH2	WAT	1055 33.615 1056 10.283	-4.295	32.761	1.00	68.91
	1553	OH2	WAT	1056 10.283 1057 28.514	0.501	-14.456	1.00	68.91
0.5	1554	OH2	WAT WAT	1057 26.514	-5.089	16.354	1.00	68.91
25	1555	OH2	WAT	1059 32.212	-2.748	2.548	1.00	68.91
	1556	OH2 OH2	WAT	1060 28.253	-14.928	-6.193	1.00	68.91
	1557 1558	OH2	WAT	1061 22.375	14.011	20.937	1.00	68.91
	1559	OH2	WAT	1062 17.962	-4.643	18.605	1.00	68.91
30	1560	OH2	WAT	1063 33.412	17.614	12.726	1.00	68.91
50	1561	OH2	WAT	1064 14.403	13.829	5.224	1.00	68.91
	1562	OH2	WAT	1065 22.334	16.845	22.648	1.00	68.91
	1563	OH2	WAT	1066 3.946	-0.489	7.854	1.00	68.91
	1564	OH2	WAT	1067 19.383	17.873	5.189	1.00	68.91
35	1565	OH2	WAT	1068 15.472	16.647	23.054	1.00	68.91
	1566	OH2	WAT	1069 29.541	28.573	2.954	1.00	68.91
	1567	OH2	WAT	1070 22.439	9.086	32.823	1.00	68.91 68.91
	1568	OH2	WAT	1071 12.994	2.582	4.613 4.759	1.00 1.00	68.91
	1569	OH2	WAT	1072 8.173	-4.098 21.529	-8.5 6 3	1.00	68.91
40	1570	OH2	WAT	1073 6.843 1074 6.493	8.743	13.308	1.00	68.91
	1571	OH2	WAT	1074 6.493 1075 38.018	4.521	-0.320	1.00	68.91
	1572	OH2	WAT WAT	1076 24.471	-3.010	18.115	1.00	68.91
	1573	OH2 OH2	WAT	1077 25.888	-4.454	10.596	1.00	68.91
45	1574	OH2 OH2	WAT	1078 14.459	7.299	-5.712	1.00	68.91
43	1575 1576	OH2	WAT	1079 29.390	19.413	11.601	1.00	68.91
	1577	OH2	WAT	1080 20.808	23,774	28.950	1.00	68.91
	1578	OH2	WAT	1081 30.321	32.666	4.517	1.00	68.91
	1579	OH2	WAT	1082 18.638	14.702	5.513	1.00	68.91
50	1580	OH2	WAT	1083 10.393	2.751	24.212	1.00	68.91
•	1581	OH2	WAT	1084 34.357	8.750	4.350	1.00	68.91
	1582	OH2	WAT	1085 38.981	27.376	6.226	1.00	68.91
	1583	OH2	WAT	1086 13.633	-5.771	10.421	1.00	68.91
	1584	OH2	WAT	1087 30.187	-0.118	1.986	1.00	68.91
55	1585	OH2	WAT	1088 19.984	12.423	13.551	1.00	68.91
	1586	OH2	WAT	1089 33.138	0.672	3.694	1.00	68.91 68.91
	1587	OH2	WAT	1090 22.605	13.264	0.581 9.575	1.00	68.91
	1588	OH2	WAT	1091 14.668	10.306	8.575 11.480	1.00 1.00	68.91
	1589	OH2	WAT	1092 21.896	16.105 0.604	11.132	1.00	68.91
60	1590	OH2	TAW	1093 26.996 1094 31.571	7.546	16.430	1.00	68.91
	1591	OH2	TAW	1094 31.571 1095 30.193	7.5 46 3.267	-18.033	1.00	68.91
	1592	OH2	TAW TAW	1095 30.193	6.862	20.521	1.00	68.91
	1593 1594	OH2 OH2	WAT	1097 25.159	32.416	11.157	1.00	68.91
	1034	0112	*****	,				

5	1595 1596 1597 1598 1599 1600	OH2 OH2 OH2 OH2 OH2 OH2	WAT WAT WAT WAT WAT WAT	1098 - 25.354 1099 - 20.969 1100 - 32.515 1101 - 30.357 1102 - 30.517 1103 - 13.656 1104 - 15.222	-13.410 -1.882 -1.311 10.302 8.184 -2.654 19.539	18.368 24.389 -2.770 -14.689 27.857 31.941 18.640	1.00 1.00 1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91 68.91 68.91
10	1601 1602 1603 1604	OH2 OH2 OH2 OH2	WAT WAT WAT	1105 34.184 1106 27.056 1107 33.492	25.830 25.512 6.985 8.497	5.139 13.333 -2.929 11.009	1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91
	1605 1606 1607 1608	0H2 0H2 0H2 0H2	WAT WAT WAT	1109 23.498 1110 29.557 1111 29.239	11.331 -10.045 18.077 12.553	13.153 18.238 -10.203 -11.333	1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91
15	1609 1610 1611 1612	OH2 OH2 OH2 OH2	TAW TAW TAW	1112 20.316 1113 27.872 1114 21.439 1115 34.052	2.853 20.739 2.985 -3.141	33.575 -11.349 36.842 18.133	1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91
20	1613 1614 1615 1616	OH2 OH2 OH2 OH2	WAT WAT WAT	1116 11.123 1117 10.985 1118 33.767 1119 23.247	13.263 28.659 24.523 23.627	12.061 -2.115 18.586 14.310	1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91
25	1617 1618 1619 1620	OH2 OH2 OH2 OH2	WAT WAT WAT	1120 31.382 1121 12.025 1122 9.969 1123 20.360	-1.649 2.385 -3.059	0.565 20.835 -13.904	1.00 1.00 1.00	68.91 68.91 68.91

15

20

As used herein, an atomic coordinate, also referred to herein as a structure coordinate or coordinate, is a mathematical coordinate derived from mathematical equations related to the patterns obtained on diffraction of X-rays by the atoms of a protein crystal. The diffraction data are typically used to calculate an electron density map, such as that shown in Fig. 1, which is used to establish the positions of the individual atoms within the unit cell of the crystal. A model that substantially represents the atomic coordinates specified in Table 1 includes not only models that literally represent the coordinates but also models representing a coordinate transformation of such atomic coordinates, for example, by changing the spatial orientation of the coordinates.

Additional embodiments of the present invention include 3-D models of extracellular domains of FceRI\alpha proteins that substantially represent the atomic coordinates specified in Table 5, Table 6, Table 7 or Table 8, each of which is at the end of the Examples section. Similarly, a model that substantially represents the atomic coordinates specified in Table 5, Table 6, Table 7 or Table 8 includes not only models that literally represent the coordinates but also models representing a coordinate transformation of such atomic coordinates.

The present invention also includes a 3-D model that is a modification of a 3-D model that substantially represents the atomic coordinates specified in Table 5, Table 6, Table 7 or Table 8. As used herein, a modification, also referred to herein as a model modification, is a model that represents a protein that binds to a Fc domain of an antibody. A model modification includes, but is not limited to: a refinement of the model that substantially represents the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8; a model representing any fragment of a protein having the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8 that binds to a Fc domain of an antibody; a model based on other FceRIa protein crystals, such as a model based on one or more of the crystals disclosed in the Examples; a model produced using homology modeling techniques to, for example, incorporate all or any part of the amino acid sequence of another FcR into a 3-D model of the extracellular domain of the model substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8 or incorporate all or any part of the amino acid sequence of a FceRIα protein into a 3-D model of another FcR; and a modification representing a FcR 30

15

30

with an altered function, which preferably can be used to design a mutein with an improved function compared to an unmodified protein. As used herein, the term unmodified protein refers to a protein that has not been intentionally subjected to either random or site-directed (i.e., targeted) mutagenesis.

A model of the present invention can be represented in a variety of forms including, but not limited to, listing the coordinates of all atoms comprising the model, providing a physical 3-D model, imaging the model on a computer screen, providing a picture of said model, and deriving a set of coordinates based of a picture of the model, for example by extracting coordinates from a picture or placing a similar immunoglobulin domain into the 3-D model of human $FeeRI\alpha_{1-176}$ protein form M1, FceRI α_{1-176} protein form M2, FceRI α_{1-172} protein form T1, FceRI α_{1-172} protein form T2, or $FceRI\alpha_{1-172}$ protein form H1 and deriving a model of the similar domain. Physical 3-D models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, Biosym Technologies, San Diego, CA, Tripos, Inc., and Molecular Simulations Inc. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Hard copies include both motion and 20 still pictures. Computer screen images and pictures of the model can be visualized in a number of formats including, but not limited to, electron density maps, ribbon diagrams, space-filling representations, α carbon traces, topology diagrams, lists of interatomic vectors, phi/psi/chi angle representations of the coordinates, and contact maps, examples of some of which are in the Figs. Representations of the model can include the entire 25 model or portions thereof.

In one embodiment, a model of the present invention identifies the solvent accessibility of amino acid residues of the corresponding protein. The solvent accessibilities of the amino acids in human $FceRIa_{1-176}$ protein (form M1) are indicated in Table 2.

Table 2. PhFceRIa₁₋₁₇₆, Form M1, residue exposure

>>>> Surface plot for:
>>>> structure file= fcr10_gen.mtf
>>>> coordinate set= fcr10b.pdb

	>>>>	Coordinate	201-10110-1-		
5	<u>resid</u>	resname	access	access-main	access-side
•				5.5920	29.2803
	4	LYS	18.7522	0.7105	0.2895
	5	PRO	0.5301	0.5227	25.5856
	6	LYS	14.4465	2.9151	0.0000
	7	VAL	1.6658	1.6199	28.7895
10	8	SER	10.6765	4,3765	2,4038
10	9	LEU	3.3901	0.9379	24.0120
	10	ASN	12.4750	0.9379 0.1896	21.0688
	11	PRO	9.1378		21.7181
	12	PRO	10.7886	2.5914	3.8672
15	13	TRP	2.8040	0.1461	5.6746
13	14	ASN	2.8382	0.0019	1.3672
	15	ARG	0.8717	0.0047	1.6524
	16	ILE	0.8262	0.0000	0.3536
	17	PHE	0.2251	0.0002	16.8470
20		LYS	10.3275	2.1781	0.0000
20	18	GLY	5.9941	5.9941	6.2230
	19	GLU	3.4574	0.0003	7.8142
	20	ASN	5.5027	3.1911	0.2464
	21	VAL	0.4139	0.5396	12.3812
	22	THR	5.3412	0.0611	0.2767
25		LEU	0.1383	0.0000	16.1931
	24	THR	6.9459	0.0105	0.0913
	25	CYS	0.2279	0.2962	10.3594
	26	ASN	6.3601	2.3608	
_	27	GLY	15.2937	15.2937	0.0000
3		ASN	12.5836	3.3134	21.8538
	29		2.9321	4.7397	1.1246
	30	ASN	10.9538	0.4808	16.9384
	31	PHE	16.8929	5.7840	23.2409
	32	PHE	19.4108	11.1422	26.0256
3	33	GLU	10.7289	4.6702	18.8072
	34	VAL	2.4235	2.0900	3.0905
	35	SER	13.8183	6.2435	28.9679
	36	SER	0.2048	0.0825	0.3679
	37	THR	11.0359	0.0996	19.7850
	40 38	LYS	0.0222	0.0000	0.0311
	39	TRP	3.1821	0.0194	4.9894
	40		3.3786	0.3964	5.3667
	41		6.4876	7.0690	5.9062
	42		10.7019	10.7019	0.0000
	45 43		11.7545	1.4355	32.3926
	44		12.7619	7.2235	18.3003
	45		5.1618	3.6359	8.2137
	46		18.9113	6.7955	28.6039
	4		5.1912	1.8435	7.8693
	50 4		10.4814	0.7172	23.5005
	4		12.2883	1.293	
	5	0 ASN	12.2003		

		_	7.5400	0.9771	20.6683
	51	SER	7.5408 5.9824	1.1729	15.6016
	52	SER	2.7 94 8	0.0000	5.5895
	53	LEU	11.0365	4.8824	17.1907
	54	ASN	1.4787	1.1377	1.8197
5	55	ILE	10.1929	3.7822	18.7406
	56	VAL	10.1929	0.9161	19.1928
	57	ASN	0.4355	0.5444	0.0000
	58	ALA	12.3709	0.0000	22.2676
	59	LYS	3.8585	0.0995	6.0065
10	60	PHE	8.4358	0.0765	15.1232
	61	GLU	3.5771	0.0000	7.1543
	62	ASP	0.1109	0.0000	0.3328
	63	SER	1.4454	1.4454	0.0000
	64	GLY	3.8623	0.1172	6.8583
15	65	GLU	0.6305	0.0000	0.9458
	66	TYR	5.0231	0.0000	9.0416
	67	LYS	0.0000	0.0000	0.0000
	68	CYS	4.0004	0.1217	7.1034
	69	GLN	1.6360	1.2124	1.9183
20	70	HIS	12.0520	6.5738	16.4346
	71	GLN	6.9718	4.8885	8.6385
	72	GLN	18.2550	4.0583	37.1841
	73	VAL	11.7258	0.8064	22.6451
	74	ASN GLU	8.0572	4.5805	10.8386
25	75	SER	1.1935	1.7903	0.0000
	76	GLU	11.7837	0.3001	20.9705
	77 70	PRO	6.8729	3.9043	10.8310
	78 70	VAL	4.7487	0.8978	9.8832
20	79	TYR	10.6722	1.0753	15.4707
30		LEU	0.6889	1.0101	0.3678
	81	GLU	6.0039	0.0005	10.8066
	82	VAL	1.1805	2.0660	0.0000
	83 84	PHE	3.1391	0.5957	4.5925
24		SER	11.3103	7.0817	19.7676
3:	86	ASP	5.0469	1.8059	8.2880
	87	TRP	8.7876	0.0000	12.3027
	88	LEU	0.2129	0.4258	0.0000 0.9408
	89	LEU	0.4967	0.0525	
A	.0 90	LEU	0.0300	0.0599	0.0000 0.3323
4	91	GLN	0.1846	0.0000	0.0495
	92	ALA	0.1116	0.1271	8.8700
	93	SER	6.6376	5.5213	28.7952
	94	ÅLA	6.8725	1.3918	11.9535
_	45 9 5	GLU	7.3784	1.6594	22.0772
_	96	VAL	11.5981	3.7388	0.9951
	97	VAL	0.8323	0.7102	22.0682
	98	MET	11.2704	0.4727	14.3246
	99	GLU	9.0020	2.3489	0.0000
	50 100	GLY	8.7203	8.7203	19.0137
	101		10.5632	0.0000	14.7788
	102		7.5364	2.1046 0.0065	0.0136
	103	LEU	0.0101	0.0000	11.9250
	104	PHE	7.5886	0.0000	0.0026
	55 105	5 LEU	0.0013	0.0005	7.8855
	100		5.0182	0.000	

			0.4000	0.1901	0.0004
	107	CYS	0.1269 0.9132	0.3845	1.2657
	108	HIS	0.5179	0.5179	0.0000
	109	GLY	4,5690	0.0000	6.3966
	110	TRP	16.0050	8.4847	20.3023
5	111	ARG	12.3469	5.3472	19.3466
	112	ASN	5.4418	2,5536	6.5971
	113	TRP	12.2436	2.6722	21.8150
	114	ASP	1.0913	1.1789	0.9745
	115	VAL	9.9588	0.0536	14.9114
10	116	TYR	15.8288	6.4497	23.3321
	117	LYS	2.4049	3.9634	0.3269
	118	VAL	7.4508	0.0000	14.9016
	119	ILE	0.0000	0.0000	0.0000
	120	TYR TYR	3.5355	0.0193	5.2936
15	121	LYS	4.6755	0.3398	8.1440
	122	ASP	10.1763	6.7061	13.6465
	123	GLY	13.3789	13.3789	0.0000
	124	GLU	13.2240	0.9044	23.0796
•	125	ALA	9.8218	3.5091	35.0725
20	126	LEU	2.8644	3.0445	2.6843
	127	LYS	20.0249	8.2304	29.4606 12.5774
	128 129	TYR	9.3305	2.8367	20.5908
	130	TRP	16.4879	6.2307	3.3740
25	131	TYR	3.4405	3.5735	19.7905
23	132	GLU	11.9086	2.0563	14.2802
	133	ASN	9.2765	4.2727	12.7321
	134	HIS	7.6393	0.0000	15.8860
	135	ASN	8.0044	0.1229	0.4205
30		ILE	0.3804	0.3402 6.1883	17.4541
50	137	SER	9.9436	0.9189	1.0252
	138	ILE	0.9720	2.3046	30.6869
	139	THR	14.4684	3.2729	22.0554
	140	ASN	12.6642	0.2930	0.0431
35		ALA	0.2430	0.0000	15.8087
-	142	THR	6.7751	1.2997	31.8640
	143	VAL	14.3987	2.9912	23.5929
	144	GLU	14.4366	0.0018	1.2841
	145	ASP	0.6429	1.9108	12.8352
4	0 146	SER	5.5523 4.1321	4.1321	0.0000
	147	GLY	• • •	0.0488	9.5879
	148	THR	4.1370 0.0265	0.0000	0.0398
	149	TYR	3.8147	0.0000	5.7220
	150	TYR	0.0000	0.0000	0.0000
4	15 15 1	CYS	3.7177	0.0000	8.6747
	152		0.4224	0.4224	0.0000
	153		6.3203	0.0000	11.3765
	154		0.0418	0.0267	0.0620
	155		11.9658	3.7888	15.2367
	50 156		15,4277	4.3561	24.2849
	157		14.1140	0.4176	27.8104
	150		13.2798	6.7381	19.8215
	15	·	4.2173	2.1486	5.2517
	16		11.5466	4.1966	17.4267
	55 16		0.5960	0.8940	0.0000
	16	Z SER	 -		

		0111	10.5746	0.2964	18.7972
	163	GLU	11.0115	3.8863	20.5117
	164	PRO	1.6740	0.6758	2.6721
	165 .	LEU		2.2692	8.1825
	166	ASN	5.2259	0.5937	0.0000
5	167	ILE	0.2968	0.0262	22.8875
	168	THR	9.8239	2.6882	0.3236
	169	VAL	1.6748		18.8869
	170	ILE	10.3926	1.8982	25.3128
	171	LYS	15.1729	2.4981	43.7220
10	172	ALA	11.6822	3.6722	
10	173	PRO	13.4157	5.3766	24.1346
	174	ARG	25.5533	20.1410	28.6460
	21A	NAG	17.8283	0.0000	17.8283
		NAG	10.6799	0.0000	10.6799
	42A	NAG	8.9040	0.0000	8.9040
15	42B	MAN	17.4386	0.0000	17.4386
	42C	*****	16.8280	0.0000	16.8280
	166A	NAG	16.9174	0.0000	16.9174
	166B	NAG	21.1827	0.0000	21,1827
	166C	MAN	21.1021	0.000	

The solvent accessibilities of the amino acids in human FceRIa protein forms T1, T2, M2 and M1 are indicated in Tables 9, 10, 11, and 12 respectively, each of which is at the end of the Examples section.

Residues that are solvent accessible are important as they represent amino acids that are on the external surface of the protein and, as such, may be involved in binding of a FcR to an antibody and as such be useful in designing proteins with an enhanced binding activity or in identifying compounds that inhibit such binding. In addition, solvent accessible residues can represent targets for modification to produce a FcR with improved function. Such analysis also identifies residues in the interior, or core, of the protein. Such residues can also be targeted to produce proteins with improved functions, such as enhanced stability. A model of the present invention also provides additional information that is not available from other sources. For example, a model can identify the crystal contacts between crystals and predict the location of the IgE binding domain, including those amino acids that actually form contacts with a Fc domain of an IgE antibody, such as those in the binding face of the FceRla protein. A model can also identify the amino acids in the interface between domain 1 and domain 2 (i.e., the D1D2 interface), as well as those in the cleft formed between the two domains.

One embodiment of the present invention is a model that represents a protein that binds to a Fc domain of an IgE antibody with an affinity that is at least equivalent to the affinity of the extracellular domain of human FcεRIα for any one of the following IgE antibodies: a human IgE antibody, a canine IgE antibody, a feline IgE antibody, an equine IgE antibody, a rat IgE antibody, and a murine IgE antibody. Such a model can represent an extracellular domain of a human FcεRIα protein, a canine FcεRIα protein, an equine FcεRIα protein, a murine FcεRIα protein, and a rat FcεRIα protein. Such a model can also represent a protein with altered substrate specificity, preferably designed based on a model of the present invention. WO 98/23964, *ibid.*, reports the ability of an isolated human FcεRIα protein to bind to canine, feline and equine IgE antibodies. Models of the present invention can be used to design a FcR with increased affinity for an antibody of a species other than self, such as, but not limited to, a human FcεRIα with increased affinity for a canine, feline or equine IgE antibody.

The present invention includes a model that represents a FcR that binds to an antibody of its respective class (i.e., IgE, IgG, IgM, IgA or IgD antibody class). Also included is a model that represents a FcR designed to bind to an antibody of a class other than the class to which the protein naturally binds. Such a model of the present invention can be produced, for example, by incorporating all or any part of the amino acid sequence of the other FcR into a 3-D model of the extracellular domain of a human FceRIa protein. Such an embodiment includes any model that specifically incorporates any Ig domains that are placed in an orientation (packing interfaces and bend angles) that is based on the structure of the FceRIa. A preferred model of the present invention represents a FcR that binds to an IgE antibody or to an IgG antibody. In one embodiment, a model of the present invention is a 3-D model of an extracellular antibody binding domain of a FcR other than human FceRIa, such as of a FcR that binds to an IgG antibody. Such proteins and models thereof can be designed by homology modeling by, for example, altering the substrate specificity of a FceRIa protein such that the altered protein binds an IgG antibody.

A preferred modified model of the present invention is a model that has a 3-D structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 10 angstrom when superimposed, using backbone atoms, on the 3-D model substantially represented by the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8, and more particularly atomic coordinates specified in Table 1. Preferably such a model has a 3-D structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 8 angstroms, preferably less than 7 angstroms, preferably less than 6 angstroms, preferably less than 5 angstroms, preferably less than 4 angstroms, preferably less than 3 angstroms, preferally less than 2 angstroms, and preferably less than 1 angstroms, when superimposed, using backbon3 atoms, on the 3-D model substantially represented by the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7, or Table 8, and more particularly atomic coordinates specified in Table 1. In this embodiment, such a model represents a FcR that binds to an antibody. The backbone atoms are those atoms that form the backbone, or 3-D folding pattern, of the model. As such, backbone atoms are the base residues of amino acids, i.e., nitrogen, carbon, the alpha carbon and oxygen.

Also preferred is a model modification having an amino acid sequence that shares at least about 30%, preferably at least about 40%, more preferably at least about 45%, more preferably at least about 50%, more preferably at least about 60% and even more preferably at least about 80% amino acid sequence homology, with a human FceRIα protein, as determined using the program ALIGN with default parameters, optimal global alignment of two sequences with no short-cuts. It is to be noted that, using the same program and parameters, the extracellular domain of a human FceRIα protein (i.e., soluble human FceRIα protein) shares about 48% identity with feline and rat soluble FceRIα proteins, about 49% with a murine soluble FceRIα protein, about 50% identity with a canine soluble FceRIα protein, and about 60% identity with an equine soluble FceRIα protein. A preferred model of the present invention represents an IgE binding domain, i.e., a region that binds to an IgE antibody.

One embodiment of the present invention is a 3-D model of a human FceRIa protein produced by a method that includes the steps of: (a) crystallizing an extracellular domain of a human FceRIa protein, such as, but not limited to a protein having amino acid sequence SEQ ID NO:2 or SEQ ID NO:4; (b) collecting X-ray diffraction data from the crystallized protein; and (c) determining the model from the X-ray diffraction data, preferably in combination with an amino acid sequence of the protein. A protein for crystal formation can be produced using a variety of techniques well known to those skilled in the art. As disclosed herein, a human FceRIa protein to be crystallized is preferably produced in recombinant insect cells transformed with a gene encoding an extracellular domain of a human FceRIa protein, such as a baculovirus genetically engineered to produce the protein. The purity of the FceRIa protein must be sufficient to permit the production of crystals that can be analyzed by X-ray crystallography to a resolution that permits determination of a 3-D model of the protein. Preferably the resolution is at least about 4 angstroms (i.e., 4 angstroms or better), more preferably at least about 3.5 angstroms, more preferably at least about 3 angstroms, more preferably at least about 2.5 angstroms, more preferably at least about 2 angstroms and even more preferably at least about 1.5 angstroms. Methods to obtain such purity levels are well known to those skilled in the art. 30

WO 00/26246

5

10

20

25

As disclosed herein, a preferred method to crystallize a FceRIa protein is by vapor distillation. Particularly preferred methods are disclosed in the Examples. It should be appreciated that the present invention also includes other methods known to those skilled in the art by which the protein can be crystallized.

-51-

3-D models of some proteins have been determined; see, for example, Blundell et al., *Protein Crystallography*, Academic Press, London, 1976. However, as discussed herein, elucidation of the crystal structure of the extracellular domain of the human FceRIa was difficult. In one embodiment, crystal structure determination includes obtaining high-resolution data using synchrotron radiation. Such data can be collected, for example, at the Stanford Synchrotron Source Laboratory, Palo Alto, CA, or the Advanced Photon Source at Argonne National Laboratories, Argonne, IL. Additional locations to collect such data include, but are not limited to, Brookhaven, NY, and Japan. In one embodiment, diffraction data from native and heavy-atom treated crystals provide an initial image of the protein structure which is refined into an electron density map. Details regarding data collection and interpretation are provided in the Examples section.

One embodiment of the present invention is a method to produce a 3-D model of a FceRI\(\alpha\) protein that includes positioning amino acid representations (i.e., representing amino acids) of the protein at substantially the coordinates listed in Table 1, Table 5, Table 6, Table 7, or Table 8. That is, knowledge of the coordinates of the protein permits one skilled in the art to produce a model of the protein using those coordinates. Such a model, or any model which is essentially represented by a simple coordinate transformation of the coordinates specified in Table 1, Table 5, Table 6, Table 7, or Table 8, can be represented in a variety of methods as heretofore disclosed and is included in the present invention.

In another embodiment, a model of the present invention can be refined to obtain an improved model, which is an example of a model modification, also referred to as a modified model. Refining methods can include, but are not limited to, further data collection and analysis; data collection from frozen crystals; introduction of solvent molecules to the structure; clarification of secondary structure; and analyses of crystallized complexes between a FcR and an antibody or inhibitory compound. An

15

30

additional model refinement method includes analyzing a 3-D model to predict amino acid residues that if replaced are likely to yield proteins with at least one improved function, effecting at least one such replacement, determining whether the activity of the modified protein agrees with the prediction, and refining the model as necessary.

Methods to determine whether the modification agrees with prediction include producing the modified protein and performing assays with that modified protein to determine if the protein does indeed exhibit the improved function(s), such as desired activity, stability and solubility properties. Assays to measure such functions are well known in the art; examples of several such assays are disclosed herein.

Another embodiment of the present invention is a modified 3-D model that represents a FcR other than a human FceRIa protein represented by the 3-D model the coordinates of which are listed in Table 1, Table 5, Table 6, Table 7, or Table 8. Preferably the amino acid sequence of the protein to be modeled is known. In such a case, the modified model can be produced using the technique of homology modeling, preferably by incorporating (e.g., grafting, overlaying or replacing) all or any portion of the amino acid sequence of the other FcR into the 3-D model of the human FccRIa protein to produce the modified model which comprises the other FcR. General techniques for homology modeling, also referred to as molecular replacement, have been disclosed in, for example, Greer, 1990, Proteins: Structure, Function, and Genetics 7, 317-334; Havel et al., 1991, J. Mol. Biol. 217, 1-7; Schiffer et al., 1990, Proteins: Structure, Function, and Genetics 8, 30-43; and Lattman, 1985, Methods Enzymol 115, 55-77. However, such technology has not been applied to FcRs since, until the present invention, no 3-D model of any FcR was available. Thus, the present invention now allows the solving of the structures of a number of other natural and mutated forms of FcRs or any other protein with significant amino acid homology, especially to the 25 functional Ig domains of the human FceRIa protein.

In one embodiment, a model of a FcR, such as, but not limited to a FccRI α protein, is produced by extracting the 3-D coordinates from a published figure or building a 3-D model with atoms from other Ig domains wherein the Ig domains are oriented as predicted for a human FccRI α_{1-176} protein or a FccRI α_{1-172} protein. For example, a model of the present invention can be produced by orienting two known Ig

15

domains into a bent confirmation similar to that of the two domains of the human FcεRIα protein. Such a model is referred to as a model in which domain 1 and domain 2 are oriented in a manner as specified by the structural coordinates listed in Table 1, Table 5, Table 6, Table 7, or Table 8. This model can then be used in further molecular replacement methods. Such methods can include the steps of (a) orienting the model by three rotations; and (b) translating the model in one to three directions to produce additional model modifications.

Suitable FcRs for which a 3-D model can be determined using homology modeling include any mammalian FcR, such as a protein that binds to IgE, IgG, IgM,

10 IgA or IgD antibodies. Preferred is a protein that binds to an IgE antibody or an IgG antibody. Preferred FcRs that bind to IgE include human, canine, feline, equine, murine and rat FcεRIα proteins. The present invention also includes the use of other Ig domains to produce models of the present invention.

One embodiment of the present invention is a 3-D model of a FcR having an improved function compared to an unmodified protein as well as a method to produce such a modified model. Such an improved function includes, but is not limited to, enhanced activity, enhanced stability and enhanced solubility. Such a modified model can be produced by replacing at least one amino acid based on information derived from analyzing the 3-D model of a FceRI α protein, such as the model of a human FceRI α_{1-176} protein or a $FceRI\alpha_{1-172}$ protein, such that the replacement leads to a protein with an improved function. As used herein, a replacement refers to an (i.e., one or more) amino acid substitution, insertion, deletion, inversion and/or derivatization (e.g., acetylation, glycosylation, phosphorylation, PEG modification, biotinylation, and covalent attachment of other ligands or other compounds to the protein. In one embodiment, synthetic chemical methods are used to produce either a fragment or the entire protein to, 25 for example, introduce non-natural amino acids or other chemical compounds into the structure of a FcR. For example, based on a structure of the present invention, one can design synthetic peptides or larger proteins that could be linked to produce an intact protein with IgE binding activity, the structure allowing one to design the start and stop points for these peptides, e.g., at surface accessible loops. In accordance with the present invention, an amino acid that is substituted or inserted can be a natural amino

20

25

acid or an unnatural amino acid, including a derivitized amino acid. Methods to identify regions in the protein that, if changed, yield a protein with an improved function are disclosed below.

The present invention includes use of a 3-D model of the present invention to identify a compound that inhibits binding between a ker and an antibody. The advantages of using a 3-D model to identify inhibitory compounds are multi-fold in that the model depicts the site at which a Fc domain of an antibody binds to its FcR, i.e., the antibody-binding domain, also referred to as the antibody binding site. As such, a large number of potential inhibitory compounds can be initially analyzed without having to perform in vitro or in vivo laboratory studies. As used herein, methods to identify inhibitory compounds include, but are not limited to, designing inhibitory compounds 10 based on the 3-D model of a FcR, probing such a 3-D model with compounds that are potential inhibitors in order to identify those compounds that are actually inhibitory of the binding of an antibody to its FcR, screening a compound data base using such a 3-D model to identify compounds that inhibit such binding, and combinations thereof. Methods to use 3-D models to design, probe for, or screen for suitable inhibitory 15 compounds are known to those skilled in the art. In particular, there are a number of computer programs that enable such methods. See, for example, PCT Publication No. WO 95/35367, by Wilson et al., published December 28, 1995.

An inhibitory compound can be any natural or synthetic compound that inhibits the binding of an antibody to a FcR. Examples include, but are not limited to, inorganic compounds, oligonucleotides, proteins, peptides, antibodies, antibody fragments, mimetics of peptides or antibodies (such as, mimetics of antibody or receptor binding sites), and other organic compounds. Compounds can inhibit binding in either a competitive or non-competitive manner and can either interact at the binding site or allosterically. An inhibitory compound should be capable of physically and structurally associating with a FcR and/or an antibody such that the compound can inhibit binding between the two entitites. As such, an inhibitory compound is preferably small and is of a structure that effectively prevents or disrupts binding. Inhibitory compounds can be identified in one or multiple steps. For example, a compound initially identified that inhibits binding between an antibody and FcR to some extent can be used as a lead to

re 1100///---

design, probe or screen for a compound with improved characteristics, such as greater efficacy, safety, solubility, etc. A preferred inhibitory compound is a compound that is efficacious when administered to an animal in an amount that results in a serum concentration of from about 1 nanomolar (nM) to 100 micromolar (µM), with a concentration of from about 10 nM to 10 μ M being more preferred.

One embodiment of the present invention is a method to identify a compound that inhibits the binding between an IgE antibody and a FceRIa protein. Such a method includes the step of using a 3-D model substantially representing the atomic coordinates specified in T_{ℓ} le 1, Table 5, Table 6, Table 7, or Table 8 to identify such a compound. Included in the present invention are inhibitory compounds that interact directly with the IgE binding domain or the receptor binding domain of the IgE antibody as well as compounds that interact indirectly with an FceRIa protein, such as compounds that interact with the D1D2 interface, with the cleft between D1 and D2, with a region not consisting of a N-linked glycosylation site, with a region suggested by a combination of 3-D model and mutagenesis analysis to indirectly affect antibody binding, a region suggested by homology with other FcERIa proteins of other species, a region suggested 15 by homology with other FcRs. In a preferred embodiment, an inhibitory compound interacts with at least one of the following regions of a model representing a FceRIa protein: a A'B loop of D1, a EF loop of D1, a BC loop of D2, a C strand of D2, a CC' loop of D2, a C'E loop of D2, a F strand of domain D2, a FG loop of D2, and a tryptophan-containing hydrophobic ridge. It is to be noted that the A'B and EF loops of 20 D1 are immediately adjacent to the IgE binding domain in D2 and as such are predicted, for the first time, by the model to be good targets for inhibitory compounds. In a preferred embodiment, an inhibitory compound of the present invention interacts with at least one amino acid that is a crystal contact as predicted by the atomic coordinates listed in Table 1, Table 5, Table 6, Table 7 or Table 8. Inhibitory compounds of the present 25 invention preferably interact with at least one of the following amino acid residues: amino acid 87, 110, 113, 115, 117, 118, 120, 121, 122, 123, 128, 129, 131, 149, 153, 154, 155, 156, 157, 158, and 159 of SEQ ID NO:2 or SEQ ID NO:4, as well as any surface residue within about 10 angstroms of any of the listed amino acids. More 30

20

25

preferred is an inhibitory compound that interacts with at least one amino acid that is a crystal contact predicted to also be part of the IgE binding domain. Particularly preferred are amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4 as well as any surface residue within about 10 angstroms of amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4. In one embodiment, an inhibitory compound of the present invention is a peptide corresponding to at least a portion of any of the identified regions or a derivative thereof, such as a peptide mimetic or other compound that mimics that peptide. Preferred is a peptide corresponding to at least a portion of the FG loop of D2, or a derivative thereof, such as a peptide mimetic or other compound that mimics that peptide.

One embodiment of a method to identify a compound that inhibits the binding between an IgE antibody and a FceRI\a protein includes the steps of: (a) generating a model substantially representing the atomic coordinates listed in Table 1, Table 5, Table 6, Table 7, or Table 8, or a model of an IgE binding domain thereof, on a computer screen; (b) generating the spacial structure of a compound to be tested; and (c) testing to determine if the compound interacts with said IgE binding domain, wherein such an interaction indicates that the compound is capable of inhibiting the binding of an IgE antibody to a FceRI\a protein. In a preferred embodiment, step (a) includes the step of identifying one or more amino acid(s) in the IgE binding domain of the model that interact directly with the Fc domain of an IgE antibody when the Fc domain binds to the IgE binding domain. Preferably a compound to be tested will interact directly with one or more of those amino acid(s). Preferred amino acids with which an inhibitory compound should interact are disclosed herein.

The present invention also includes inhibitory compounds isolated in accordance with the methods disclosed herein. Methods to produce such compounds in quantities sufficient for use, for example, as protective agents (e.g., preventatives or therapeutics) are known to those skilled in the art. It should also be appreciated that it is within the scope of the present invention to expand the use of models of the present invention to produce models of any suitable FcRs (i.e., model modifications) and to identify compounds that inhibit the binding of antibodies to such FcRs.

30

The present invention also includes use of a 3-D model of the present invention to rationally design and construct modified forms of FcRs that have one or more improved functions, such as, but not limited to, increased activity, increased stability and increased solubility compared to an unmodified FcR. Muteins of the present invention include full-length proteins as well as fragments (i.e., truncated versions) of such proteins.

One embodiment of the present invention is a FcR that comprises a mutein that binds to a Fc domain of an antibody. Such a mutein has an improved function compared to a protein comprising SEQ ID NO:2 or SEQ ID NO:4. Examples of such an improved function include, but are not limited to, increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility. Such a mutein can be produced by a method that includes the steps of: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7, or Table 8 to identify at least one amino acid of the protein represented by the model which if replaced by a specified amino acid would effect the improved function of the protein; and (b) replacing the identified amino acid(s) to produce a mutein having the improved function. Knowledge of the coordinates allows one to target specific residues, e.g. in the hydrophobic core or on the surface, to generate an accessible set of variants that can then be selected for a particular property, e.g. high stability, high affinity, altered substrate specificity, or other desirable properties (i.e., improved functions). Without the coordinates, one would have to analyze an 20 extraordinarily large number of variants, e.g., on the order of ~1011 possibilities. The structure, in contrast, allows one to pick the most relevant residues for selecting a desired property by, for example, phage display or other methods. In a preferred embodiment, replacement of one or more amino acids does not substantially disrupt the 3-D structure of the protein; i.e., the modified protein, or mutein, is still capable of 25 binding to the Fc domain of an antibody. A preferred mutein is a FcR that binds to a Fc domain of an IgE antibody, although the invention also covers muteins binding to other classes of antibodies.

In one embodiment, a mutein of the present invention has increased stability compared to its unmodified counterpart. As used herein, increased stability refers to the

25

ability of a mutein to be more resistant, for example, to higher or lower temperature, to more acidic or basic pH, to higher or lower salt concentrations, to oxidation and/or reduction, to deamidation, to other forms of chemical degradation and to proteolytic degradation compared to unmodified FcR. Increased stability can also refer to the ability of a mutein of the present invention to be stable for a longer period of time either during storage (i.e., to have a longer shelf life) or during use (i.e., to have a longer half-life under reaction conditions) than does an unmodified protein. Muteins of the present invention can also exhibit a decreased entropy of unfolding, thereby stabilizing the proteins. Increased stability can be measured using a variety of methods known to those skilled in the art; examples include, but are not limited to, determination of melting temperature, thermal denaturation, pressure denaturation, enthalpy of unfolding, free 10 energy of the protein, or stability in the presence of a chaotropic agents such as urea, guanidinium chloride, guanidinium thiocyanate, etc. A preferred mutein of the present invention has a melting temperature substantially higher than that of an unmodified FcR. Preferably the melting temperature of a mutein is at least about 1°C higher, and more preferably at least about 10°C higher than the melting temperature of the corresponding unmodified protein. Also preferred is a mutein having binding activity over a pH range that is at least about 1 pH unit higher and/or lower than the active pH range of the corresponding unmodified protein.

Another embodiment of the present invention is a mutein that exhibits increased affinity for a Fc domain of an antibody compared to its unmodified counterpart. As used herein, a mutein having increased affinity is a FcR that exhibits a higher affinity constant (K_A) or lower dissociation cometant (K_D) than its unmodified counterpart. Such a higher affinity constant can be achieved by increasing the association rate (k,) between the mutein and the Fc domain and/or decreasing the dissociation rate (k_d) between the mutein and the Fc domain. A preferred mutein of the present invention has a KA for a Fc domain of at least about 3 x 109 liters/mole (M-1), which is equivalent to a K_D of less than or equal to about 3.3 x 10⁻¹⁰ moles/liter (M). More preferred is a mutein having a K_A for a Fc domain of at least about 2 x 10^{10} M⁻¹, and even more preferably of at least about 1 x 10¹¹ M⁻¹. Also preferred is a mutein having a k₁ for a Fc domain of at least about 1 x 10⁵ liters/mole-second as well as a mutein having a k_d for a Fc domain of less 30

25

than or equal to 3 x 10⁻⁵/second. More preferred is a mutein having a k_a for a Fc domain of at least about 3 x 10⁵ liters/mole-second, and even more preferably of 1 x 10⁶ liters/mole-second. Also preferred are muteins having a k_d for a Fc domain of less than or equal to 1 x 10⁻⁵/second or even more preferably less than or equal to 3 x 10⁻⁴/second. A preferred Fc domain is that of an IgE antibody. Methods to measure such binding constants is well known to those skilled in the art; see, for example, Cook et al., 1997, *ibid.*, which reports the following values for the binding of human FcεRIα protein to human IgE: k_{a1} of 3.5 (±0.9) x 10⁵ M⁻¹s⁻¹; k_{a2} of 8.6 (±3.5) x 10⁴ M⁻¹s⁻¹; k_{d1} of 1.2 (±0.1)

x 10⁻² s⁻¹; k₄₂ of 3.2 (±0.8) X 10⁻⁵ s⁻¹; K_{A1} of 2.0 X10⁷ M⁻¹; K_{A2} of 2.9 X10⁹ M⁻¹.

Another embodiment of the present invention is a mutein that exhibits altered substrate specificity compared to its unmodified counterpart. A mutein exhibiting altered substrate specificity is a mutein that binds with increased affinity to a Fc domain of an antibody class or antibody species of a different type than that normally bound by its unmodified counterpart. In one embodiment, a mutein of a human FcεRIα protein with altered substrate specificity is a FcR that binds with increased affinity to a IgE antibody of another mammal, such as, but not limited to, a canine, feline, equine, murine, or rat IgE antibody. In another embodiment, a mutein of a human FcεRIα protein with altered substrate specificity is a FcR that binds with increased affinity to an antibody of another class, such as IgG, IgM, IgA, or IgD, with IgG being preferred.

Such a mutein can also show altered species substrate specificity. Methods to determine whether a mutein exhibits altered substrate specificity are well known to those skilled in the art.

Yet another embodiment of the present invention is a mutein that exhibits increased solubility compared to its unmodified counterpart. Such a protein is less likely to form aggregates. Methods to determine whether a mutein exhibits increased solubility are well known to those skilled in the art.

As disclosed herein, the 3-D model representing a FceRI α protein is advantageous in determining strategies for producing muteins having an improved function, e.g., for identifying targets to modify in order to obtain muteins having improved functions. Examples of targets are as follows. A key feature of the human FceRI α_{1-176} protein or the FceRI α_{1-172} protein is the crystal contacts in five space groups,

a subset of which are predicted to interact directly with a Fc domain of an IgE antibody. Such contacts are included in the IgE binding domain which is unique for human FceRIa in that the domain includes a tryptophan-containing hydrophobic ridge positioned on the top face of the crystal structure (i.e., amino acids W87, W110, W113, and W156 of SEQ ID NO:2 or SEQ ID NO:4) and an FG loop comprising amino acids from 155 to 158 of SEQ ID NO:2 or SEQ ID NO:4 that protrudes above the interface in an unusual manner. Another key feature is the interface between domain 1 and domain 2 (i.e., the D1D2 interface) which includes amino acids 12, 13, 14, 15, 16, 17, 18, 20, 84, 85 and 86 in D1 and 87, 88, 89, 90, 91, 92, 93, 95, 104, 106, 108, 110, 111, 161, 163, 164, and 165 in D2 of SEQ ID NO:2 or SEQ ID NO:4. Also important are the two domains themselves: D1 includes amino acids 1 through 86 of SEQ ID NO:2 or SEQ ID NO:4; and D2 includes amino acids 87 through 176 of SEQ ID NO:2 or amino acids 87 through 172 of SEQ ID NO:4. Another important feature is the cleft between D1 and D2, which can be identified using the coordinates. Other areas of interest include the hydrophobic core which can be identified using the coordinates, the A'B loop of D1, which includes 15 amino acids 18 and 19, the EF loop of D1, which includes amino acids 59-63, the BC loop of D2, which includes amino acids 110-114, the C strand of D2, which includes amino acids 114-123, the CC' loop of D2, which includes amino acids 123-125, the C'E loop of D2, which includes amino acids 127-134, in the different confirmations observed in the five crystal forms, and the F strand of D2, which includes amino acids 147-155 of SEQ ID NO:2 or SEQ ID NO:4. Yet another striking feature is the finding that the amino and carboxyi termini of the human $FceRIa_{1-176}$ protein are only 10 angstroms apart.

In accordance with the present invention, a mutein having an improved function can be produced by a method that includes replacing at least one amino acid based on 25 information derived from analyzing a 3-D model of the present invention to produce the mutein having the improved function. Knowledge of the structure of the extracellular domain of a human FceRIa protein crystal, for example, permits the rational design and construction of modified forms of the protein by permitting the prediction and production of substitutions, insertions, deletions, inversions and/or derivatizations that effect an improved function. That is, analysis of 3-D models of the present invention

25

provide information as to which amino acid residues are important and, as such, which amino acids can be changed without harming the protein. In making amino acid replacements, it is preferred to use amino acid replacements that have similar numbers of atoms and that allow conservation of salt bridges, hydrophobic interactions and 5 hydrogen bonds unless the goal is to purposefully change such interactions. The 3-D structure of the human FceRIa protein suggests that large deletions may not be desirable, particularly due to the relation between the various domains of the protein and the observation that most of the structure is well ordered in the crystal. An exception to this is the non-constrained loops of D1, which apparently could be deleted or shortened without harming the protein's function. These loops span amino acids 31-35 and 70-74 of SEQ ID NO:2 or SEQ ID NO:4.

It is to be appreciated that although one amino acid replacement capable of improving the function of a protein can substantially improve that function, more than one amino acid replacement can result in cumulative changes depending on the number and location of the replacements. For example, although one amino acid replacement capable of substantially increasing the stability of a protein can increase the melting temperature of that modified protein by about 1°C, about 5 to about 6 replacements may increase the melting temperature of the resultant protein by about 10°C.

In accordance with the present invention, the 3-D model of the human FceRIa protein has been analyzed, using techniques known to those skilled in the art, to determine the accessibility of the amino acids represented within the model to solvert. Such information is provided in, for example, Table 2, Table 9, Table 10, Table 11, and Table 12.

A number of methods can be used to produce muteins of the present invention. One method includes the steps of: (a) analyzing a 3-D model substantially representing the coordinates specified in Table 1, Table 5, Table 6, Table 7, or Table 8 to identify at least one amino acid of the modeled protein which if replaced by a specified amino acid would effect an improved function; and (b) replacing the identified amino acid(s) to produce a mutein having that improved function. In one embodiment, a method to produce a mutein includes the steps of (a) comparing a key region of a model of a human 30 FcεRIα protein with the amino acid sequence of a FcR having an improved function

compared to the unmodified FceRIa protein in order to identify at least one amino acid segment of the FcR with the improved function that if incorporated into the FcRI α protein represented by the model would give the FceRIa protein the improved function; and (b) incorporating the segment into the FceRIa protein, thereby providing a mutein with the improved function. In another embodiment, a method to produce a protein includes the steps of: (a) using a model representing a human FceRIa protein to identify a 3-D arrangement of residues that can be randomized by mutagenesis to allow the construction of a library of molecules from which a improved function can be selected; and (b) identifying at least one member of the mutagenized library having the improved function. In one example, a mutein is produced by a method that includes the steps of: (a) effecting random mutagenesis of nucleic acid molecules encoding a target of a 10 FCERIa protein as identified by analyzing a model of that protein, such as an IgE binding domain; (b) cloning such mutagenized nucleic acid molecules into a phage display library, wherein said phage display library expresses the target; and (c) identifying at least one member of the library that expresses a target with an improved function, such as an antibody binding domain exhibiting increased affinity for an antibody. As stated 15 above, the model allows the use of this technique in a straightforward manner that could not be accomplished in the absence of the model. It is to be also noted that these methods can also be used with other models of the present invention to produce muteins of the present invention. 20

The present invention includes a number of methods, based on analysis of a 3-D model of the present invention, to replace (i.e., add, delete, substitute, invert, derivatize) at least one amino acid residue in the protein represented by the model in order to produce a mutein of the present invention. Such methods include, but are not limited to:

25 (a) replacing at least one amino acid in at least one non-constrained loop of domain 1 in an area proximal to the FceRI gamma chain putative binding site; (b) joining an amino-terminal amino acid residue to a carboxyl-terminal amino acid residue of an extracellular domain of a FceRIα protein; (c) replacing at least one amino acid site with an amino acid suitable for derivatization; (d) replacing at least one pair of amino acids of the protein with a cysteine pair to enable the formation of a disulfide bond that stabilizes the protein; (e) removing at least a portion of the region between the B strand and C strand

30

of domain 1; (f) removing at least a portion of the region between the C strand and E strand of domain 1; (g) replacing at least one amino acid in the IgE binding domain in order to increase the affinity between an IgE antibody and the protein; (h) replacing at least one amino acid of the protein with an amino acid such that the replacement decreases the entropy of unfolding of the protein; (i) replacing at least one asparagine or glutamine of the protein with an amino acid that is less susceptible to deamidation than is the amino acid to be replaced; (j) replacing at least one methionine, histidine or tryptophan with an amino acid that is less susceptible to an oxidation or reduction reaction than is the amino acid to be replaced; (k) replacing at least one arginine of the protein with an amino acid that is less susceptible to dicarbonyl compound modification than is the amino acid to be replaced; (1) replacing at least one amino acid of the protein susceptible to reaction with a reducing sugar sufficient to reduce protein function with an amino acid less susceptible to that reaction; (m) replacing at least one amino acid of the protein with an amino acid capable of increasing the stability of the inner core of the protein; (n) replacing at least one amino acid of the protein with at least one N-linked glycosylation site; (o) replacing at least one N-linked glycosylation site of the protein 15 with at least one amino acid that does not comprise an N-linked glycosylation site; and (p) replacing at least one amino acid of the protein with an amino acid that reduces aggregation of the protein.

Amino acid replacements can be carried out using recombinant DNA techniques known to those skilled in the art, including site-directed mutagenesis (e.g., oligonucleotide mutagenesis, random mutagenesis, polymerase chain reaction (PCR)-aided mutagenesis, gapped-circle site-duceted mutagenesis) or chemical synthetic methods of a nucleic acid molecule encoding the desired protein, such as, but not limited to a human FceRIa protein, followed by expression of the mutated gene in a suitable expression system, preferably an insect, mammalian, bacterial, yeast, insect, or mammalian expression system. See, for example, Sambrook et al., *ibid*.

One embodiment of the present invention is a mutein in which at least one amino acid in at least one non-constrained loop of a FceRI α protein is replaced in order to improve a function of the protein. Finding that the human FceRI α protein had such loops was surprising, and it is believed, without being bound by theory, that a mutein in

which at least a portion of at least one such loop is replaced, would at least exhibit enhanced stability. In a preferred embodiment, at least a portion of one or more of such loops is (are) deleted. Preferred loops to replace are in domain 1 (i.e., spanning amino acids 31-35 and 70-74 of SEQ ID NO:2 or SEQ ID NO:4), preferably in an area

proximal to the FceRI gamma chain putative binding site, i.e., the site on the FceRIα protein to which the gamma chain of the high affinity Fc epsilon receptor is thought to bind. In a preferred embodiment, one or more amino acids is replaced to make loops shorter, but including 1 or 2 hydrophobic residues to pack toward the protein interior and at least one hydrophilic residue to maintain solubility.

Another embodiment of the present invention is a mutein of the extracellular 10 domain of a FceRIa protein in which an N-terminal (amino-terminal) amino acid residue is joined, preferably covalently, to a C-terminal (carboxyl-terminal) amino acid residue in order to improve a function of the protein. Finding that the N-termini and C-termini of the human FceRIa protein were only 10 angstroms apart was quite surprising. Without being bound by theory, it is believed that such a mutein would at least exhibit 15 enhanced stability. Furthermore, a covalent linker used to join the termini could also include a substance useful, for example, to anchor a mutein on a surface, as would be useful, for example, in a diagnostic assay, or to label the mutein. For a protein consisting of SEQ ID NO:2, a preferred N-terminal residue is an amino acid residue at position 1, 2, or 3 of SEQ ID NO:2, and a preferred C-terminal residue is an amino acid 20 residue at position 174, 175, or 176 of SEQ ID NO:2. Covalent linkage can be accomplished by methods known to those skilled in the art, such as, but not limited to, adding one or more N-terminal and C-terminal cysteines and crosslinking them with chemical compounds, adding additional residues in the coding sequence to allow the formation of a disulfide bond, or adding one or more lysines and coupling them through 25 a 10 angstrom linker, and including non-natural amino acid analogues by synthetic methods or by a combination of biosynthetic and organosynthetic methods. Examples of a substance to add to a covalent linker includes: ligands useful in allowing for the attachment of a mutein to a surface, such as biotin and related compounds, avidin and related compounds, metal binding compounds, sugar binding compounds, 30 immunoglobulin binding domains, and other tag domains; and detectable markers, such

15

as enzyme labels, physical labels, radioactive labels, fluorescent labels, chemiluminescent labels, and chromophoric labels. Examples include, but are not limited to, alkaline phosphatase, horseradish peroxidase, digoxygenin, luciferase, other light-generating enzymes and magnetic beads. It is also to be noted that ligands can function as detectable markers.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid suitable for derivatization. Muteins in which at least one amino acid is replaced with an amino acid suitable for derivatization include proteins that are chemically modified (e.g., a lysine already existing on the protein is modified) as well as those in which an amino acid residue is replaced with a different amino acid residue (e.g., a glycine with a lysine) as well as proteins to which a substance is added, preferably to the amino or carboxyl terminus of the protein. Examples of such substances include ligands and detectable markers as disclosed above. Preferable amino acids to replace include residues that are solvent exposed (e.g., those listed in Table 2, Table 9, Table 10, Table 11, or Table 12), but that are preferably not within about 10 angstroms of the IgE binding domain. In one embodiment, a glycosylation site, or other solvent exposed site, is replaced with a charged or polar residue to increase solubility or create more stable muteins. Glycosylation sites in human FceRIa protein include amino acids 21, 42, 50 74, 135, 140, and 166 of SEQ ID NO:2 or SEQ ID NO:4. A preferred amino acid to use as a replacement, or to chemically modify directly, includes a cysteine 20 or a lysine, with a cysteine being preferred. Compounds to use in chemical derivatizations are known to those skilled in the art; cysteines can, for example, be derivatized with maleimides.

Another embodiment of the present invention is a mutein in which a pair of amino acids have been replaced with a cysteine pair in order to improve the function of 25 the mutein, at least by increasing stability. Cysteine pairs can be substituted into a FcεRIα protein at any two residue positions identified with available programs and algorithms that would allow the formation of an undistorted disulfide bridge. In one embodiment, a serine and lysine near the termini of the protein is each replaced with a cysteine. In another embodiment, cysteine pairs are replaced with other amino acids, 30 such as serines to eliminate non-essential disulfide bonds.

30

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced in the region between the B strand and C strand of domain 1 and/or the region between the C and E strand of domain 1. In a preferred embodiment, at least a portion of such a region is deleted.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced in the IgE binding domain in order to increase the affinity between an IgE antibody and the protein. Preferred residues to replace are in or near the IgE binding domain, or IgE binding site, as determined by analysis of the 3-D model. Such residues are preferably within about 10 angstroms of residues identified by mutagenesis and further shown by model to be in an IgE binding site. Examples of such 10 residues include amino acids 87, 110, 113, 115, 117, 118, 120, 121, 122, 123, 128, 129, 131, 149, 153, 154, 155, 156, 157, 158, and 159 of SEQ ID NO:2 or SEQ ID NO:4, and amino acids within 10 angstroms of such listed amino acids. In one embodiment, preferred amino acids to replace include amino acids 87, 115, 117, 118, 120-123, 128, 129, 131, 149, 153, 155 and 159 of SEQ ID NO:2 or SEQ ID NO:4 as well as any surface residue within about 10 angstroms of any of the listed amino acids, with amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4 as well as any surface residue within about 10 angstroms of amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4 being particularly preferred. It is to be noted that amino acids 115, 118, 120, 131, 149 and 155 of SEQ ID NO:2 or SEQ ID NO:4 are buried, and 20 that amino acids that are partially buried or glycine include residues 122, 129 and 153. Additional amino acid residues to target include those in the A'B loop of D1, and EF loop of D1. Note that these residues are not the same as those shown in mutation studies to affect IgE binding since some of those mutants have mutations in amino acids that are internal to the protein; this finding can only be made by analysis of a model of the 25 present invention.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid capable of increasing the stability of the inner core or surface of the protein. Preferred amino acids to replace are hydrophilic residues located in the hydrophobic core of the protein and/or hydrophobic amino acids at the protein surface that are not within about 10 angstroms of the IgE binding domain

25

residues of D1 or D2. Preferred amino acids to replace into the hydrophobic core are hydrophobic residues such as, but not limited to, tryptophan, leucine, isoleucine, valine and alanine, as well as space filling amino acids, such as other aromatic amino acids. Preferred amino acids to replace onto the surface are polar amino acids, such as, but not limited to, glutamic acid, glutamine, aspartic acid, asparagine, histidine and serine. Muteins having one or more such amino acid replacements would exhibit at least increased stability and/or reduced aggregation. Additional preferred amino acid replacements are those that introduce salt bridges at the protein surface to stabilize protein folds. It is noted that the cysteines at positions 26 and 68 of SEQ ID NO:2 or SEQ ID NO:4 form a disulfide bond in domain 1 that is somewhat exposed to solvent, depending especially on the conformation of the D1 "30 loop" (i.e., amino acids 31-35 of SEQ ID NO:2 or SEQ ID NO:4). In one embodiment, changes in neighboring residues can be made in, for example, residues 1-5, 27-37, 49-52, or 69-75, to bury this disulfide from exposure to solvent. For example, phage display of receptors with randomized mutations in the 30 loop, might be useful for selecting receptors that react 15 less well with reducing reagents and have a more stable D1 core.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid that decreases the entropy of unfolding of the protein. The entropy of unfolding of a protein can be measured and compared to that of another protein using techniques known to those skilled in the art. A number of methods known to those skilled in the art can be used to reduce the number of protein conformations possible in the unfolded state, thereby improving the ability of the protein to fold correctly. One embodiment of the present invention for decreasing the entropy of unfolding includes replacing at least one amino acid of the protein with a specified amino acid in order to maintain certain desirable phi and psi backbone conformation angles in the protein; see, for example, PCT International Publication No. WO 89/01520, by Drummond et al., published February 23, 1989. For example, a proline residue in a protein constrains the backbone conformation to certain restricted angles. Analysis of a 3-D model of a protein of the present invention permits the identification of candidate replacement positions in the protein that have the conformation expected for a proline, but that do not have a proline in them. Such knowledge is used to

20

25

30

introduce prolines into such candidate replacement positions to "anchor" the resultant mutein in the desired conformation. The 3-D model also permits the identification of candidate replacement sites that if replaced with a proline do not substantially disrupt the 3-D structure of the resultant protein. Similarly, glycines in appropriate positions can be replaced with an amino acid having a β carbon atom or a branched β carbon atom, preferably an alanine, in order to stabilize the backbone of the protein.

Another embodiment of the present invention is a mutein in which at least one asparagine or glutamine is replaced with an amino acid that is less susceptible to deamidation. Preferred amino acids to replace include solvent accessible asparagines and glutamines.

Another embodiment of the present invention is a mutein in which at least one methionine, histidine or tryptophan is replaced with an amino acid that is less susceptible to an oxidation or reduction reaction. Preferred amino acids to replace include M98, H70, and H41. It would not be preferred to replace any of the tryptophans, nor H108 or H134 of SEQ ID NO:2 or SEQ ID NO:4.

Another embodiment of the present invention is a mutein in which at least one arginine is replaced with an amino acid that is less susceptible to dicarbonyl compound modification. Although R174 could be changed, it would probably not be preferable to change amino acids at the D1D2 interface or near the IgE binding site, such as amino acids 15, 106, or 111 of SEQ ID NO:2.

Another embodiment of the present invention is a mutein in which at least one amino acid that is susceptible to reaction with a reducing sugar sufficient to reduce protein function is replaced with an amino acid that is less susceptible to such a reaction. For example, lysines, glutamines and asparagines that could react with a sugar, such as galactose, glucose or lactose can be replaced with non-reactive amino acids.

Another embodiment of the present invention is a mutein in which one or more N-linked glycosylation sites are added to or removed from the protein, preferably by substitution with an appropriate amino acid. A FceRIa protein with additional N-linked glycosylation sites is more soluble. The ability to design a FceRIa protein having fewer, or no, N-linked glycosylation sites is also valuable as production of such a protein from production run to production run is likely to be more uniform. One embodiment is a

20

25

FceRIα mutein with no N-linked glycosylation sites that is stable, active, and soluble. Such a protein has an advantage of being produced in E. coli at low cost. In one embodiment, one or more exposed hydrophobic amino acids are changed to charged residues that form salt bridges to stabilize the protein fold and make it soluble. It is to be noted that the glycosylation sites that appear to be most often observed in the different crystal structures in the same conformation are the carbohydrate attached to positions 42 and 166 of SEQ ID NO:2 or SEQ ID NO:4. The carbohydrate attached to position 42 always appears to cover the phenylalanine at position 60 of SEQ ID NO:2 or SEQ ID NO:4. As such, one embodiment of the present invention is to remove the glycosylation site at position 42, e.g., by substitution with a suitable amino acid. This embodiment has the additional advantage that the resultant mutein has an exposed phenylalanine at position 60, thereby leading to increased IgE binding activity.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid that reduces aggregation and increases solubility of the protein, such as, for example, replacing one or more hydrophobic residues on the surface with one or more hydrophilic residues. Other examples of such amino acids to replace are disclosed herein.

Another embodiment of the present invention to enhance stability is the addition of polyethylene glycol (PEG) groups to a FcR protein, i.e., to produce a "pegylated" FcR protein. In one embodiment, the PEG group(s) can substitute for carbohydrate group(s) due to removal of one or more N-glycosylation sites. Such PEG group(s) can be attached to easily modifiable residues, such as cysteines or lysines, on the surface of the protein, such residues identifiable by analysis of a 3-D model of the present invention.

Another embodiment of the present invention is a mutein that comprises a FcR having a substance, such as a ligand or detectable marker, attached to an amino acid of the protein such that the substance does not substantially interfere with the antibody binding activity of the protein. The substance is attached in such a manner that the substance is also capable of performing its function, such as binding to a second member of a ligand pair or enabling detection of the protein. The FcR to which a substance is attached can be either an unmodified protein or a mutein of the present invention. Suitable attachment sites can be identified using 3-D models of the present invention.

15

20

25

30

Preferred attachment sites include solvent exposed amino acids, such as those listed in Table 2, Table 9, Table 10, Table 11, or Table 12. Substances can be attached, or conjugated, to the protein using techniques known to those skilled in the art. It is to be appreciated that a preferred method to attach a substance to an amino acid is to modify that amino acid to have a reactive attachment site, such as is present on cysteine and lysine amino acids. As such, an attachment site comprising a solvent exposed amino acid refers to the nature of the amino acid prior to any modification required for attachment. Examples of suitable substances to attach to a Fck include any compound capable of binding to or reacting with another substance, such as those described for attachment to a covalent linker.

It is to be appreciated that muteins of the present invention can include amino acids which are not modified because they would negatively impact the function of the protein. Such amino acids can be identified using a 3-D model of the present invention.

It should also be appreciated that it is within the scope of the present invention to expand the use of models of the present invention to produce models of and make modifications to any suitable FcRs or other Ig domain-containing proteins to produce muteins having a desired function.

The present invention also includes nucleic acid molecules that encode muteins of the present invention as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Methods to produce such proteins are also disclosed herein.

The present invention includes an isolated FcεRIα protein that consists of SEQ ID NO:2, i.e., PhFcεRIα₁₋₁₇₆. Also included in the present invention is a protein consisting of an extracellular domain of a FcεRIα protein that is structurally homologous to an isolated FcεRIα protein consisting of SEQ ID NO:2. As used herein, a protein that is structurally homologous to PhFcεRIα₁₋₁₇₆ is a protein that (a) includes both D¹ and D2 domains, (b) shares at least about 30%, and preferably at least about 40%, amino acid sequence identity with SEQ ID NO:2, as determined using a ALIGN with default parameters, optimal global alignment of two sequences with no short-cuts, (c) displays a substantially equivalent affinity for an IgE antibody as does a complete extracellular domain of the corresponding FcεRIα protein, and (d) produces crystals having sufficient

quality to enable structure determination. Examples of such proteins include a human FcεRIα protein having SEQ ID NO:4, i.e., PhFcεRIα₁₋₁₇₂ and a human FcεRIα protein having an amino acid sequence that spans from amino acid 3 through amino acid 174 of SEQ ID NO:2, i.e., PhFc ϵ RI α_{3-174} . It is to be noted that these examples are provided to 5 clarify the definition of a structurally homologous FcεRIα protein and are not intended to limit the scope of such proteins. That is, a FceRIa protein that is structurally homologous to PhFceRI α_{1-176} is any mammalian FceRI α protein having the listed characteristics. Preferred are human, canine, feline, equine, murine and rat proteins that are structurally homologous to PhFceRI α_{1-176} . Also included herein are nucleic acid molecules to encode such proteins as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Methods to produce such proteins are also disclosed herein. Preferably such proteins are produced in insect cells.

PCT/USYYI4040

The present invention also includes a FceRIa protein consisting of SEQ ID NO:4 except that the isoleucine at position 170 has been replaced by a cysteine. Also included in the present invention is a protein consisting of an extracellular domain of a FceRI α protein that is structurally homologous to an isolated FceRIa protein consisting of SEQ ID NO:4 except that the isoleucine at position 170 has been replaced by a cysteine.

15

20

25

30

The present invention also includes the following novel structures as identified by a 3-D model of the present invention: a crystal contact cluster, preferably involved in IgE binding; a tryptophan-containing hydrophobic ridge; a FG loop in D2; a D1D2 interface; a cleft between D1 and D2; a domain 1; a domain 2; a hydrophobic core; a A'B loop of D1; a EF loop of D1; a BC loop of D2; a C strand of D2; a CC' loop of D2; a C'E loop of D2; and a strand of D2. Also included herein are nucleic acid molecules to encode such structures as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Also included are methods to produce such structures and models thereof.

The present invention also includes isolated nucleic acid molecules encoding proteins of the present invention, including, but not limited to, proteins comprising unmodified extracellular domains of FcRs, novel structures within such proteins, and muteins. As used herein, an isolated nucleic acid molecule encoding a protein is a nucleic acid molecule that has been removed from its natural milieu. As such, "isolated"

15

20

does not reflect the extent to which the nucleic acid molecule has been purified. An isolated nucleic acid molecule can be DNA, RNA, or derivatives of either DNA or RNA.

A nucleic acid molecule encoding a mutein of the present invention can be produced by mutation of parental protein genes (e.g., unmodified or previously modified protein-encoding genes, or portions thereof) using recombinant DNA techniques heretofore disclosed or by chemical synthesis. Resultant mutein nucleic acid molecules can be amplified using recombinant DNA techniques known to those skilled in the art, such as PCR amplification or cloning (see, for example, Sambrook et al., ibid.), or by chemical synthesis. A mutein can also be produced by chemical modification of a protein expressed by a nucleic acid molecule encoding an unmodified protein or muteinencoding gene.

Proteins of the present invention can be produced in a variety of ways, including production and recovery of recombinant proteins and chemical synthesis. In one embodiment, a protein of the present invention is produced by culturing a cell capable of expressing the protein under conditions effective to produce the protein, and recovering the protein. A preferred cell to culture is a recombinant cell that is capable of expressing the protein, the recombinant cell being produced by transforming a host cell with one or more nucleic acid molecules of the present invention. Transformation of a nucleic acid molecule into a host cell can be accomplished by any method by which a nucleic acid molecule can be inserted into a cell. Transformation techniques include, but are not limited to, transfection, electroporation, microinjection, lipofection, adsorption, and protoplast fusion. A recombinant cell may remain unicellular or may grow into a tissue, organ or a multicellular organism. Transformed nucleic acid molecules of the present invention can remain extrachromosomal or can integrate into one or more sites within a chromosome of a host cell in such a manner that their ability to be expressed is retained. 25

Suitable host cells to transform include any cell that can be transformed. Host cells can be either untransformed cells or cells that are already transformed with at least one nucleic acid molecule. Host cells of the present invention can be endogenously (i.e., naturally) capable of producing a protein of the present invention, but such cells are not preferred. Host cells of the present invention can be any cell that when transformed with a nucleic acid molecule of the present invention are capable of producing a protein of the

10

15

20

present invention, including bacterial, yeast, other fungal, insect, animal, and plant cells. Preferred host cells include bacterial, yeast, insect and mammalian cells, and more preferred host cells include Escherichia, Bacillus, Saccharomyces, Pichia, Trichoplusia, Spodoptera and mammalian cells. Particularly preferred host cells are Trichoplusia ni cells, Spodoptera frugiperda cells, and Chinese hamster ovary cells.

A recombinant cell is preferably produced by transforming a host cell with a recombinant molecule comprising a nucleic acid molecule of the present invention operatively linked to an expression vector containing one or more transcription control sequences. The phrase operatively linked refers to insertion of a nucleic acid molecule into an expression vector in a manner such that the molecule is able to be expressed when transformed into a host cell. As used herein, an expression vector is a DNA or RNA vector that is capable of transforming a host cell, of replicating within the host cell, and of effecting expression of a specified nucleic acid molecule. Expression vectors can be either prokaryotic or eukaryotic, and are typically viruses or plasmids. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including in bacterial, yeast, other fungal, insect, animal, and plant cells. Preferred expression vectors of the present invention can direct gene expression in bacterial, yeast, insect and mammalian cells.

Nucleic acid molecules of the present invention can be operatively linked to expression vectors containing regulatory control sequences such as promoters, operators, repressors, enhancers, termination sequences, origins of replication, and other regulatory control sequences that are compatible with the host cell and that control the expression of the nucleic acid molecules. In particular, recombinant molecules of the present invention include transcription control sequences. Transcription control sequences are sequences which control the initiation, elongation, and termination of transcription. Particularly important transcription control sequences are those which control 25 transcription initiation, such as promoter, enhancer, operator and repressor sequences. Suitable transcription control sequences include any transcription control sequence that can function in at least one of the recombinant cells of the present invention. A variety of such transcription control sequences are known to those skilled in the art. Preferred 30

5

transcription control sequences include those which function in bacterial, yeast, insect and mammalian cells.

It may be appreciated by one skilled in the art that use of recombinant DNA technologies can improve expression of transformed nucleic acid molecules by manipulating, for example, the number of copies of the nucleic acid molecules within a host cell, the efficiency with which those nucleic acid molecules are transcribed, the efficiency with which the resultant transcripts are translated, and the efficiency of posttranslational modifications. Recombinant techniques useful for increasing the expression of nucleic acid molecules of the present invention include, but are not limited to, operatively linking nucleic acid molecules to high-copy number plasmids, integration of the nucleic acid molecules into one or more host cell chromosomes, addition of vector 10 stability sequences to plasmids, substitutions or modifications of transcription control signals (e.g., promoters, operators, enhancers), substitutions or modifications of translational control signals (e.g., ribosome binding sites, Shine-Dalgarno sequences), modification of nucleic acid molecules of the present invention to correspond to the codon usage of the host cell, deletion of sequences that destabilize transcripts, and use of 15 control signals that temporally separate recombinant cell growth from recombinant protein production during fermentation. The activity of an expressed recombinant protein of the present invention may be improved by fragmenting, modifying, or derivatizing nucleic acid molecules encoding such a protein. 20

In accordance with the present invention, recombinant cells can be used to produce proteins by culturing such cells under conditions effective to produce such a protein, and recovering the protein. Lefective conditions to produce a protein include, but are not limited to, appropriate media, bioreactor, temperature, pH and oxygen conditions that permit protein production. An appropriate medium refers to any medium in which a cell of the present invention, when cultured, is capable of producing the protein. An effective medium is typically an aqueous medium comprising assimilable carbohydrate, nitrogen and phosphate sources, as well as appropriate salts, minerals, metals and other nutrients, such as vitamins. The medium may comprise complex nutrients or may be a defined minimal medium. Cells of the present invention can be cultured in conventional fermentation bioreactors, which include, but are not limited to, 30

10

20

batch, fed-batch, cell recycle, and continuous fermentors. Culturing can also be conducted in shake flasks, test tubes, microtiter dishes, and petri plates. Culturing is carried out at a temperature, pH and oxygen content appropriate for the recombinant cell. Such culturing conditions are well within the expertise of one of ordinary skill in the art.

Depending on the vector and host system used for production, resultant proteins may either remain within the recombinant cell; be secreted into the fermentation medium; be secreted into a space between two cellular membranes, such as the periplasmic space in E. coli; or be retained on the outer surface of a cell or viral membrane. The phrase "recovering the protein" refers simply to collecting the whole fermentation medium containing the protein and need not imply additional steps of separation or purification. Proteins of the present invention can be purified using a variety of standard protein purification techniques, such as, but not limited to, affinity chromatography, ion exchange chromatography, filtration, electrophoresis, hydrophobic interaction chromatography, gel filtration chromatography, reverse phase chromatography, chromatofocusing and differential solubilization. 15

The present invention also includes isolated (i.e., removed from their natural milieu) antibodies that selectively bind to a FcR of the present invention (i.e., anti-FcR antibodies). As used herein, the term "selectively binds to" FcR refers to the ability of antibodies of the present invention to preferentially bind to specified proteins of the present invention. Binding can be measured using a variety of methods standard in the art including enzyme immunoassays (e.g., ELISA), immunoblot assays, etc.; see, for example, Sambrook et al., ibid. Isolated antibodies of the present invention can include antibodies in a bodily fluid (such as, but not limited to, serum), or antibodies that have been purified to varying degrees. Antibodies of the present invention can be polyclonal or monoclonal. Functional equivalents of such antibodies, such as antibody fragments and genetically-engineered antibodies (including single chain antibodies or chimeric antibodies that can bind to more than one epitope) are also included in the present invention. Antibodies can be produced using methods known to those skilled in the art. A preferred method to produce antibodies of the present invention includes (a) administering to an animal an effective amount of a protein of the present invention to produce the antibodies and (b) recovering the antibodies. In another method, 30

20

25

antibodies of the present invention are produced recombinantly using techniques as heretofore disclosed to produce proteins of the present invention. Antibodies raised against defined proteins can be advantageous because such antibodies are not substantially contaminated with antibodies against other substances that might otherwise cause interference in a diagnostic assay or side effects if used in a therapeutic composition.

Antibodies of the present invention have a variety of potential uses that are within the scope of the present invention. Examples of such uses are disclosed in WO 98/27208, ibid., see, for example, page 24.

A FcR of the present invention can include chimeric molecules comprising at least a portion of a FcR that binds to an antibody and a second molecule that enables the chimeric molecule to be bound to a substrate in such a manner that the antibody receptor portion binds to the antibody in at least as effective a manner as a FcR that is not bound to a substrate. An example of a suitable second molecule includes a portion of an immunoglobulin molecule or another ligand that has a suitable binding partner that can be immobilized on a substrate, e.g., biotin and avidin, or a metal-binding protein and a metal (e.g., His), or a sugar-binding protein and a sugar (e.g., maltose).

The present invention includes uses of proteins, antibodies and inhibitory compounds of the present invention for the diagnosis and treatment of allergy and the regulation of other immune responses in an animal.

One embodiment is a therapeutic composition comprising at least one of the following therapeutic compounds: an inhibitory compound of the present invention, a mutein of the present invention, or an antibody of the present invention. Also included is a method to protect an animal from allergy or other abnormal immune responses. Such a method includes the step of administering a therapeutic composition of the present invention to the animal. As used herein, the ability of a therapeutic composition of the present invention to protect an animal from allergy or other abnormal immune responses refers to the ability of that composition to, for example, treat, ameliorate or prevent allergy or other abnormal immune responses. General characteristics of therapeutic compositions and methods to produce and use such therapeutic compositions are disclosed, for example, in WO 98/27208, ibid., see, for example, page 39-47. It is to 30

be noted that although the compositions and methods disclosed in WO 98/27208, *ibid.*, relate to feline FcεRIα proteins, they are also applicable to therapeutic compositions of the present invention. Therapeutic compositions of the present invention are advantageous because they can be derived from analysis of 3-D models of the present invention and have improved functions, such as efficacy and safety.

Another embodiment is a diagnostic reagent comprising a mutein of the present invention. As used herein, a diagnostic reagent is a composition that includes a mutein that is used to detect allergy or other abnormal immune responses in an animal. Also included in the present invention are methods, including in vivo methods and in vitro methods, to (a) detect allergy or other abnormal immune response, or susceptibility thereto, in an animal, comprising use of a diagnostic reagent comprising a mutein of the present invention and (b) to enhance the performance of an IgE binding assay, said method comprising incorporating into the assay a mutein of the present invention. General characteristics of diagnostic reagents and methods to produce and use such diagnostic reagents are disclosed, for example, in WO 98/27208, ibid., see, for example, page 2-39. It is to be noted that although the reagents and methods disclosed in 15 WO 98/27208, ibid., relate to feline FcεRIα proteins, they are also applicable to diagnostic reagents, kits and detection methods of the present invention. Muteins of the present invention are advantageous in such applications because of their enhanced affinity for antibodies, altered specificity, enhanced solubility and/or enhanced stability, 20 enabling for example use in otherwise adverse conditions and longer shelf-life.

The following examples are provided for the purposes of illustration and are not intended to limit the scope of the invention.

EXAMPLES

Example 1

5

10

30

This Example describes the production of a FceRIa nucleic acid molecule, a recombinant molecule, a recombinant cell, a recombinant virus, and a FceRIa protein of the present invention.

A number of human FceRIα proteins of variable lengths (i.e., 171, 172, and 176 amino acids) were produced in a variety of cell lines (i.e., Chinese hamster ovary cells, *Pichia pastoris* yeast, *Spodoptera frugiperda* (Sf9) insect cells and *Trichoplusia ni* (Hi-5) insect cells). Due to a number of factors, however, including protein length, solubility, and extent and variability of glycosylation, only one FceRIα protein was useful in producing a crystal of sufficient quality for the first determination of a model of an extracellular domain of a FceRIα protein. The production of this protein is disclosed below.

A nucleic acid molecule comprising the first 176 amino acids of the mature form of the human FcεRIα protein, nucleic acid molecule and protein designated herein as nhFcεRIα₁₋₅₂₈ and PhFcεRIα₁₋₁₇₆, respectively, was produced as follows. An *Eco*RI-HindIII fragment from plasmid EdpC20 (Blank et al., *ibid.*) containing the human FcεRIα signal sequence and residues 1-172 of the mature human FcεRIα protein was ligated to two oligonucleotides coding for residues 172-176 of the mature protein and two stop codons. The two oligonucleotides, having nucleic acid sequences of 5' AGCTCCGCGT GAGAAGTAAT AAG 3' (SEQ ID NO:5) and 5' GATCCTTATT ACTTCTCACG CuG 3' (SEQ ID NO:6), had *Hin*dIII and *Bam*HI overhangs when annealed together, which permitted the ligation of nhFcεRIα₁₋₅₂₈ into *Eco*RI and *Hin*dIII cleaved baculovirus transfer vector pVL1392 (available from Pharmingen, San Diego, CA) to produce recombinant molecule pVL1392-nhFcεRIα₁₋₅₂₈. The resultant construct was verified by DNA sequencing.

Recombinant virus was produced as follows. Recombinant molecule pVL1392-nhFceRI $\alpha_{1.528}$ was co-transfected with a linear Baculogold baculovirus DNA (available from Pharmingen) into *S. frugiperda* Sf9 cells to form recombinant cell *Sf*9:pVL1392-nhFceRI $\alpha_{1.528}$ which was cultured to produce recombinant virus, namely BV:pVL1392-nhFceRI $\alpha_{1.528}$ using techniques known to those skilled in the art. Supernatants of

20

30

transfected Sf9:pVL1392-nhFceRIa₁₋₅₂₈ cells were amplified once in TNM-FH medium (available from Pharmingen), followed by a second amplification in serum-free medium (SF-900, available from Gibco, Gaithersburg, MD) in a final volume of about 500 milliliters (ml). For Sf9:pVL1392-nhFceRIa₁₋₅₂₈ cells grown in shaker flasks, TNM-FH medium was supplemented with pluronic F-68 (available from Pharmingen). For each virus stock used in protein production, the optimal amount of virus and harvest time post-infection was determined by small scale tests in 50 ml shaker flasks.

Recombinant protein PhFceRIa₁₋₁₇₆ was produced as follows. Trichoplusia ni (Hi-5) cells were infected with recombinant virus BV:pVL1392-nhFcεRIα₁₋₅₂₈ that had been produced as described above to produce recombinant cell Hi-5:pVL1392nhFcεRIα₁₋₅₂₈. Recombinant cell Hi-5:pVL1392-nhFcεRIα₁₋₅₂₈ was grown in shaker or spinner flasks for production of PhFcεRIα₁₋₁₇₆. Typical yields of PhFcεRIα₁₋₁₇₆ were about 2 to 12 milligrams per liter (mg/liter) of infected cells 2 to 4 days after infection.

Recombinant protein PhFcεRIα₁₋₁₇₆ was purified as follows. Supernatants from 1.5 to 5 liters of recombinant Hi-5:pVL1392-nhFceRIa₁₋₅₂₈ cells were collected, filtered through 0.2 micron filters, and loaded directly onto a Mab15-1 (Sechi et al., 1996, J. Biol. Chem. 271, 19256-19263) monoclonal antibody column. Supernatants were recirculated over the column at least twice, followed by buffer (100 millimolar (mM) Na, K phosphate, pH 7) washes of about 300 ml, until the absorbance at 280 nanometers (nm) of the eluant returned to zero. PhFceRIa₁₋₁₇₆ was eluted by two urea washes: 100 ml of 5 molar (M) urea in 100 mM phosphate, pH 7.0; then 100 ml of 7 M urea in 100 mM phosphate, pH 7.0; followed by extensive regeneration with 100 mM Na, K phosphate, pH 7.0. The urea eluants were pooled concentrated to about 25 to 40 ml with an Amicon stirring concentrator, and dialyzed 4 times against 2 liters of 50 mM Tris, pH 7.5. The purity of PhFceRI α_{1-176} was verified by SDS-PAGE. Purified PhFceRI α_{1-176} was stored 25 at 4°C in the presence of 0.05% sodium azide. Final yield of PhFceRIa₁₋₁₇₆ was about 50% based on an absorption coefficient of 2.6 mg⁻¹ml for the purified protein and the initial total protein estimated using ELISA assays with the initial cell supernatants.

An inhibition-ELISA assay was used to quantitate PhFceRIa₁₋₁₇₆ expression and yields in initial transfected supernatants, subsequent viral amplifications and large scale protein preparations. In this assay, the binding of Mab15-1 antibody to the plated

PhFceRIα₁₋₁₇₆ protein was monitored using a goat anti-mouse-alkaline phosphatase antibody (A-2429, available from Sigma, St. Louis, MO). Unknown samples were used to compete for antibody binding and compared with a standard curve generated in parallel. Fifty microliters (ml or mL) of purified PhFceRIa₁₋₁₇₆ was incubated in microtiter plates overnight at 4°C at a concentration of 1 mg/ml in phosphate-buffered saline. Plates were rinsed with wash buffer containing 20 mM Hepes, pH 7.5, 100 mM NaCl, 0.1% Tween-20 (Hepes/NaCl buffer) and blocked with Hepes/NaCl buffer containing 1% Carnation dry milk. Standard inhibitor samples ranging from 0.1-50 mg/ml of FhFceRIa₁₋₁₇₆ in two-fold dilution series ware incubated with Mab15-1 (0.1 mg/ml final concentration) and added in duplicate to wells coated with PhFceRIa₁₋₁₇₆. Standard controls included wells without overnight incubation with PhFceRIa₁₋₁₇₆, and addition of Mab15-1 without inhibiting PhFceRIa₁₋₁₇₆. Secondary antibody in a 1:5000 dilution was incubated after washing for 12 hour at room temperature. Plates were washed and developed using the AP reagent p-nitrophenyl phosphate (PNPP, available from Sigma 104-105). Microplates were read using a Molecular Devices SpectraMax Plus reader at 405 nm.

Example 2

10

15

20

25

This Example describes the production of a FceRIa protein crystal of the present invention.

Purified PhFc ϵ RI α_{1-176} , produced as described in Example 1, was concentrated to a final concentration of 20 mg/ml in 20 mM Tris pH 7.5. Crystallization was carried out using the hanging drop method, with a precipitant composed of 100 mM Tris, pH 8.5, 200 mM NaOAc, and 18-24% PEG 4000. Crystals were obtained in 2 to 10 days amidst significant amounts of protein precipitate. At lower PEG concentrations, a different crystal form was observed. The crystals used in the structure determination typically grow as clusters of 3 to 20 crystals that could be separated manually. The crystals belong to the monoclinic space group C2, with cell dimensions of 88.6 x 69.6 x 49.3 angstroms, alpha=gamma=90 degrees, beta=116.7 degrees, with one receptor molecule per asymmetric unit. Such crystals diffracted to a resolution of about 2.4 angstroms. Crystals were harvested into harvest buffer containing 35% PEG 4000, 100 mM Tris pH

30 8.5. It is to be noted that the inventors produced and tested several hundred crystals using the various other proteins described in Example 1, before successfully obtaining the crystal described immediately above.

Example 3

10

20

25

30

This Example describes the production of additional FceRIa protein crystals of the present invention.

Nucleic acid molecule nhFcεRIα₁₋₅₁₆, encoding the first 172 amino acids of the human FcεRIα protein was expressed in *T. ni* Hi-5 cells to produce PhFcεRIα₁₋₁₇₂ in a manner similar to that described for the production of PhFcεRIα₁₋₁₇₆ in Example 1. Purified PhFcεRIα₁₋₁₇₂ was concentrated to a final concentration of 20 mg/ml in 20 mM Tris pH 7.5. Crystallization was carried out using the hanging drop method, with a precipitant composed of 0.1-0.2 M NaAcetate, 0.1M Na Citrate, pH 5.6, 18-24% PEG, and HECAMEG detergent at it's Critical Micelle concentration (19.5 mM). Crystals were obtained in 2 to 10 days amidst significant amounts of protein precipitate. The crystals belong to the monoclinic space group P6122 with unit cell dimensions of 58 x 58 x 226 angstroms, alpha=beta=90 degrees; gamma=120 degrees, with one receptor molecule per asymmetric unit. Such crystals diffracted to a resolution of about 3.2 angstroms.

Using a different protocol, purified PhFczRIa₁₋₁₇₆, produced as described in Example 1, was concentrated to a final concentration of 10 mg/ml in 20 mM Tris pH 7.5. Crystallization was carried out using the hanging drop method, with a precipitant composed of 100 mM Tris, pH 7.5, 0-20% isopropanol, and 18-24% PEG 4000. Crystals were obtained in 2 to 10 days amidst significant amounts of protein precipitate. The crystals belong to the monoclinic space group C2, with cell dimensions of 136.02 x 75.01 x 79.28 angstroms, alpha=gamma=90 degrees; beta=117.8 degrees. Such crystals diffracted to a resolution of abent 3.0 angstroms.

Example 4

This Example describes the production of a three-dimensional model of the present invention.

For data collection, crystals, produced as described in Example 2, were mounted in nylon loops (available from Hampton-Research, Laguna Niguel, CA) and rapidly cooled in liquid nitrogen after a short (about 30 second) soak in harvest buffer

supplemented with 14% glycerol. Heavy atom soaks with K₂PtBr₄ and K₃AuCl₃ were done in harvest buffer with 5 mM Pt for 48 hours and 1 mM Au for 18 days. Data were collected at the Stanford Synchrotron Radiation Laboratories (SSRL) 7-1 beamline and at the Dupont-Northwestern-Dow undulator beamline at the Advanced Photon Source at Argonne National Laboratories. The statistics for these data are shown in Table 3.

Table 3. Crystallographic data and model refinement

	MOTE.	SANCE SEE	
Resolution	2.4Å	3.0Å	4.0Å
Wavelength/Energy (Å/keV)	1.08/11.48	1.02/12.12	1.05/11.76
Completeness, % (Last Shell)	96.9 (92.5)	99.9 (100.0)	96.3 (69.9)
Ave. Redundancy (Last Shell)	3.9 (3.4)	7.6 (7.3)	6.2 (2.7)
Rmerge, % (last shell)	5.7 (22.6)	10.1 (39.8)	5.1 (7.0)
<i sl=""> (last shell)</i>	23.8 (4.5)	19.0 (3.9)	35.2 (15.9)
DF/F (Resolution)	-	0.218 (20-3Å)	0.093 (20-4Å)
No. of sites	-	1	1
Phasing Power acentric/centric	-	1.50/1.93	0.41/0.61
Rcullis acentric/centric	-	0.66/0.70	0.94/0.97

Overall Figure of Merit

= 0.487

20 FOM after DM =

30

0.673

Refinement Statistics: 500-2.4Å

Reflections (free) = 10247 (880) Rfactor/Rfree, % 24.2/27.1 = #atoms 1620 = #waters 126 **RMSD** bonds 0.0077Å RMSD angles 1.53° Ave. B 65.7Å²

 R_{warp} =SII₁-<I>VSIII, where I₁ is the intensity of and individual reflection and <I> is the average intensity of that reflection.

 $R_{cayst} = SIF_pI-IF_cI/SIF_pI$, where F_c is the calculated and F_p is the observed structure factor amplitude. Phasing Power = F_{beak}/E , where F_{beak} = the heavy atom structure factor amplitude and E = the residual lack of closure error.

 $R_{cullle} = SllF_{ph} \pm F_{p}l - lF_{beale}l/SlF_{ph} \pm F_{p}l, \text{ where } F_{ph} \text{ is the derivative structure factor amplitude.}$

For the Pt and Au datasets, the wavelength was chosen to be 200 eV above the absorption edge of the metal, in order to maximize the anomalous signal for each heavy atom. Heavy atom data were collected using reverse beam protocols to optimize the anomalous diffraction signal. Diffraction data were collected with a Mar300 Image plate (SSRL) or a MarCCD detector (DND-CAT), and integrated and scaled with DENZO/SCALEPACK; see, Otwinowski et al., 1997, In Methods in Enzymology:

Macromolecular Crystallography, part A, Academic Press, pp 307-326. The CCP4 suite of programs (Collaborative Computational Project, 1994, Acta Cryst. D50, 760-763) was used for further processing and identification of heavy atom sites.

10 Heavy atom positions were identified from peaks in the anomalous and isomorphous difference patterson maps. Heavy atom positions were refined and phases calculated with the program MLPHARE, followed by solvent flattening and density modification with the program DM (Collaborative Computational Project, 1994, ibid.). The subsequent model was using the CNS program (Brunger et al., 1998, Acta Crystallogr D Biol Crystallogr 54, 905-921) with the combined maximum likelihood and experimental phase target (MLHL). Specifically, the structure of the FceRIa protein PhFceRIa₁₋₁₇₆ was determined by multiple isomorphous replacement using gold and platinum heavy atom derivatives with the anomalous signal from both derivatives. The data collection and heavy atom phasing statistics are shown in Table 3. The MIRAS phases were used as input to the density modification program DM and the electron 20 density map was of sufficient quality that the entire model except for two flexible loops and five residues at the termini could be built; see Fig. 1A and 1B. The model was further improved by cycles of automated refinement using the program CNS followed by manual rebuilding. The current R-factor and Rfree are 24.2% and 27.1% respectively for 25 all the data to 2.4 angstroms. No electron density was observed for three residues at the N-terminus (1-3) and 2 residues at the C-terminus (175-176), and poor density was observed for two loops (residues 32-35 and 70-73) that are disordered in the crystal. Final statistics for the model are shown in Table 3.

Example 5

This Example describes the structure of a FcεRIα protein predicted by a threedimensional model of the present invention.

30

A. Overall structure

The model of extracellular domain of the human FceRIa protein, also referred to herein as the hFceRIa model or hFceRIa structure, indicates that PhFceRIa is composed of two immunoglobulin (Ig) domains, D1 and D2, each about 85 residues in length, that are bent at an acute angle relative to each other and form an extended convex surface; see Fig. 2. The domain arrangement generates a flat surface at the top of the receptor that has been implicated in binding to the Fc domain of an igE antibody. The domains are small compared to canonical variable and constant Ig domains and the shorter sequence is accommodated by truncation of the CC'E crossover region; see Fig. 2. Both domains D1 and D2 of the hFceRIa model are composed of beta-strands AA'BCC'EFG, differing from the previously described I-set domains (Harpaz et al., 1994, J. Mol. Biol. 238, 528-539) by the absence of strand D. The nearly antiparallel domain packing places the A'B, CC' and EF loops of D1 and the BC, C'E and FG loops of D2 near the top of the receptor; see Fig. 2. One feature of the topology is a crossover 15 of the A strand from the ABE sheet to the CC'FG sheet, forming a short segment of parallel beta sheet in an otherwise antiparallel structure; see Fig. 2 and Fig. 3. In D1, the AA' crossover make contacts in the D1D2 interface (see below), while in the D2

Significant structural differences are also observed between D1 and D2 of the hFceRI\(\alpha\) model. The D1 and D2 sequences contain about 28% identical residues and superimpose with an RMS deviation of 1.2 angstroms for the Ca atoms. The F-G strands and loop differ between the two domains. In D2, these strands are longer and the FG loop projects above the D2 domain surface. The C' strands also differ between the two domains. In D2, a series of aromatic residues (tyrosines at positions 120 and 131) form a hydrophobic core that pushes the C' strand and loop away from the C strand, altering the local conformation of this region. The FG loop and C-C' strands of D2 form part of the binding site for IgE (see below).

domain, residues in the A strand interact with D1; see Fig. 3.

The tertiary packing arrangement of the hFceRI\alpha D1 and D2 domains is distinct from other tandem Ig domain structures; see Fig. 4. Comparison of the hFceRI\alpha model with other bent two-Ig domain structures reveals a high degree of variability in the bend angles and packing surfaces between domains. A subset of D1 and D2 representative

15

20

30

structures of are shown in Fig. 4, including those from human FceRIa (designated as IgE-FcR), the natural killer cell inhibitory receptor, (KIR, Fan et al., 1997, Nature 389. 96-100), the human growth hormone receptor (HGHBP, de Vos et al., 1992, Science 255, 306-312), the interleukin-1 receptor, (IL1R, Vigers et al., 1997, Nature 386, 190-194) and the insect defense protein hemolin (Su et al., 1998, Science 281, 991-995). The structures are oriented similarly with respect to the carboxyl-termini of the two Ig domains being compared. The figures on top show side views and the figures below show top views. The FceRIa and hemolin structures have the most acute angles relating two sequential Ig domains. The top view of these domains shows that the orientation of the hemolin and FceRIa domains are more closely related, but between this selected subset of proteins there is significant variability in the relative orientations of tandem Ig domain structures. The bend angle between domains and domain packing interfaces are clearly unique, and this variation is likely to be important in ligand binding interactions. For example, the FG loop of D2 in hFceRIa is oriented quite differently with respect to D1 residues as compared to the same region of the KIR or HGHBP, thus changing the spatial relationships of D1D2 loops that may be involved in ligand interactions. To the inventors' knowledge, the hFceRIa structure defines a new group of two sequential Ig domain structures that differs from other known tertiary arrangements.

B. The D1D2 interface

The bent shape of the FceRIα structure produces a large interface between the D1D2 domains that buries 1280 Ų of accessible surface area of 28 D1D2 residues. There are 11 residues from the D1 domain (12-18, 20, 84-86) and 17 residues from the D2 domain that are buried at the interface (87-93, 95, 104, 106, 108, 110-111, 161, 163-165). Of these 28 residues, 8 are completely conserved in all human FcgR and FceRIα sequences (corresponding to residues 13, 87, 88, 90, 91, 106, 108, 1:0 of SEQ ID NO:2); see Fig. 5. These conserved residues form a significant fraction to one side of the buried interface, suggesting that related FcRs would have a similar acute packing of the D1D2 domains as observed in the FceRIα model.

However, 20 residues that form the D1D2 interface in the FcεRIα model differ in other FcRs and these differences could alter the relative orientations of the two domains. For example, the conserved tryptophan at position 110 packs against a phenylalanine at

15

20

25

30

position 17 of FceRIα. In related FcRs, this phenylalanine is changed to a leucine, which may lead to slight alterations in the packing of the two domains. Another central residue in the FceRIα D1D2 interaction is residue R15, which forms a hydrogen bond with the carbonyl of L90 and is packed against L89, F84, and L165. In related human FcRs, arginine 15 is changed to serine or asparagine, which corresponds to a significant volume and charge change at the center of the D1D2 interaction. Since the interactions of the FcR with antibody are near the D1D2 interface, alterations in residues at the interface might influence receptor specificity. Other residues that are variable amongst the FcR sequences in the region of the D1D2 could also perturb the D1D2 interactions.

The bent hFceRIα structure generates a cleft between the two domains that is near the trans-membrane anchor at the C-terminus of D2; see Fig. 2. This cleft is located far from the IgE binding site identified by mutagenesis studies (see below). Although there is no known function attributed to this region, while not being bound by theory, it is believed that this region could be a site of interaction with the extracellular regions of the beta or gamma subunits of the receptor. It has been suggested that interactions between the FcgRI and FcgRIIIA alpha and gamma subunits increase the binding affinity of the receptor for IgG (Miller et al., 1996, *J. Exp. Med. 183*, 2227-2233). Although the extracellular regions of the human FceR gamma chain are short (about 5 to 7 amino acids), these regions could potentially interact with the D1D2 cleft and thereby affect the affinity of the receptor for antibody. In addition, recent binding studies with recombinant, soluble FceRIα and IgE have demonstrated a 10-fold lower affinity than had previously been determined in cell-binding assays (Cook et al., 1997, *ibid.*).

C. Carbohydrate attachment sites

The human FceRIα protein PhFceRIα₁₋₁₇₆ is the most highly glycosylated protein structure solved by X-ray crystallography to date, having seven N-linked glycosylation sites in 176 amino-acid residues. The intact FceRIα on mast cells is approximately 40% carbohydrate by weight (Kanellopoulos, et al., 1980, E. J. Biol. Chem. 255, 9060-9066); LaCroix, et al., 1993, ibid.), with a heterogeneous molecular weight on SDS-PAGE gels of about 50 kilodaltons (kD). Human FceRIα expressed in insect cells has a molecular weight of about 34 kD as observed using SDS-PAGE, but, based on typical insect cell glycosylation structures (-GlcNAc₂-Man₃-GlcNAc), could be expected to have a

10

25

molecular weight of about 27.5 kD, suggesting the protein is about 30% carbohydrate by weight. While the presence of carbohydrate at the seven N-glycosylation sites is not required for binding to IgE (Letourneur et al., 1995, *ibid.*; Robertson, 1993, *ibid.*; Scarselli et al., 1993, *ibid.*), mutation of these sites or treatment of FceRI-expressing cells with tunicamycin leads to the aggregation of the receptor during biosynthesis.

In the hFcεRIα structure, carbohydrate density is observed at three of the seven predicted glycosylation sites. For two of these sites, asparagines 42 and 166, three sugar moieties were built. The carbohydrate at position 42 extends up towards the top of the FcεRIα structure, covering residues F60, S63 and V83. The carbohydrate attached to position 166 projects away from the protein surface, potentially as a result of crystal contacts and the modification of the third and sixth positions of the first GlcNac residue. The third carbohydrate attachment site is the arginine at position 21.

Many of the related FcR proteins are also highly glycosylated proteins and the glycosylation sites vary between receptors. Rat and mouse FcεRIα proteins each have six potential N-linked glycosylation sites, of which two sites and one site, respectively are shared in common with the human FcεRIα protein. Comparison of seventeen human and animal FcR sequences identifies twenty-five different potential N-linked carbohydrate attachment sites in related FcRs. The twenty-five sites are distributed evenly between D1 and D2, with fourteen sites in D1 and eleven sites in D2. Five of these sites are relatively well conserved sites in all FcRs (found in > 9/17 sequences analyzed) and they correspond to residues 35, 42, 61, 135, and 142 of SEQ ID NO:2. These sites cover a significant fraction of the FcεRIα surface on both major faces of D1 and D2, placing limitations on the surface available for interactions with antibody.

It is not known why FcRs are so heavily glycosylated. Many potential roles for carbohydrate sites on proteins have been suggested, including specific roles in determining the tertiary (Wyss et al., 1995, Science 269, 1273-1278) or quaternary structures of proteins (Huber et al., 1976, Nature 264, 415-420; Vaughn et al., 1998, Structure 6, 63-73). In the case of the human FcRs, the number of potential N-linked glycosylation sites correlates to some degree with the affinity of the FcR for immunoglobulin. Table 4 shows the number of glycosylation sites in the domains corresponding to the extracellular domain of the human FcεRIα protein along with the

total number of glycosylation sites in parentheses. Affinity data are taken from Ravetch et al., 1998, *ibid.*; Ravetch et al., 1991, *Annu. Rev. Immunol.* 9, 457-492.

Table 4. Comparison of the number of predicted glycosylation sites and the affinity of different FcRs for antibody.

	iion	(CHOS)(L	a Nimity
		(idea)	
		<u>Human</u>	
	FceRI	7	high (10 ⁻⁹ -10 ⁻¹⁰ M)
5	FcyRIA (CD64)	5 (7)	high (3 domains, 10 ⁻⁸ -10 ⁻⁹ M)
	FcyRIB (CD64)	5 (7)	high (3 domains, 1) ⁻⁸ -10 ⁻⁹ M)
	FcyRIIA (CD32)	2 (3)	low (10 ⁻⁶ M)
	FcyRIIB (CD32)	3	low (10 ⁻⁶ M)
	FcyRIIC (CD32)	3 (4)	low (10-6M)
0.	FcyRIIIA (CD16)	5 (6 in variant)	low (10 ⁻⁶ M)
		Mouse	
	FceRI	6	high (10 ⁻⁹ -10 ⁻¹⁰ M)
	FcγRI	4(5)	high (3 domains, 10 ⁻⁷ -10 ⁻⁸ M)
	FcγRIIb	4(5)	low (10 ⁻⁶ M)
	FcγRIIIa	4	low (10 ⁻⁶ M)
		Rat	
5	FceRI	7	high (10 ⁻⁹ -10 ⁻¹⁰ M)
	FcγRII	6 (7 total)	low
	FcγRIII	5	low
		Other	
	FcγRII (guinea pig)	5(6)	low
	FcγRIII (pig)	3	low
20	FcyRII (bovine)	6	low

10

15

20

25

30

In the high affinity FcRs, there are typically 5 to 7 potential N-linked glycosylation sites, whereas in the low affinity FcRs there are as few as two sites. One significant difference in the function of the high and low affinity FcRs is the probability that they will bind antibody in the absence of antigen. The high affinity receptors such as FceRI can bind IgE prior to interacting with antigens. While not being bound by theory, it is believed that since FcR activation requires crosslinking of receptors, glycosylation might prevent the aggregation of large antibodies at the cell surface bound by FcRs. Crystallization of proteins at lipid/water interfaces can occur readily, and the potentially high local concentrations of membrane-bound antibodies might lead to FcR activation in the absence of antigen. The low affinity IgG receptors interact with antibody-antigen aggregates that can simultaneously bind and activate multiple FcRs. While not being bound by theory, it is believed that glycosylation may not be quite as important for these receptors, since interaction with the antibody could occur after the binding of antigen.

However, it is likely that there are additional explanations for the glycosylation that is observed in the FcRs. The non-human FcRs do not show an obvious correlation of the number of carbohydrate sites and FcR affinity. While not being bound by theory, it is believed that glycosylation might be important in FcR signaling, by orienting receptor:antibody complexes into functional signaling complexes (i.e. by preventing antigen-crosslinked complexes from forming non-functional aggregates). It is known that activation through FceRI is sensitive to some geometrical constraints imposed by antigen crosslinkers, although the nature of these physical constraints is poorly understood. The recent crystal structure determination of an erythropoietin-receptor complex suggests that the orientation of ligand-mediated dimerization of cell-surface receptors may be important in efficient signal transduction (Syed et al., 1998, *Nature* 395, 511-516).

D. Receptor binding site for IgE (IgE binding domain)

A number of mutagenesis studies have been carried out in an effort to elucidate the regions of the FceRI that are critical for the interaction with IgE molecules (Cook et al., 1997, *ibid.*; Hulett et al., 1993, *ibid.*; Hulett et al., 1994, *ibid.*; Hulett et al., 1995; Mallamaci et al., 1993, *ibid.*). These experiments have demonstrated an important

15

role for amino acids in the D2 domain of the receptor, although some regions of D1 are also likely to be involved in IgE binding. Studies suggesting that D1 plays a role in IgE binding include the deletion of D1 (Robertson, 1993, *ibid.*; Scarselli et al., 1993, *ibid.*) or substitution with a homologous IgG receptor (Hulett et al., 1994, *ibid.*). These experiments do not determine conclusively whether D1 interacts directly with the IgE or whether D1 indirectly alters the structure of D2 and subsequent interactions with IgE. Analysis of the hFceRIa model of the present invention is needed to predict important IgE binding regions in the protein. For example, the substitution or elimination of residues at the D1D2 interface can influence D2 interactions with antibody Fc regions.

In addition, there are a number of regions of D1 which have been excluded as determinants of the specificity of the receptor for IgE, since these FcεRIα segments can be substituted by the corresponding residues in the FcgRIIIA protein (Mallamaci et al., 1993, *ibid.*). These residues include segments 25-38, 43-54, 67-79, and 77-86. Substitution of residues 10-21 or 55-67 disrupt the binding of IgE and 5 different monoclonal antibodies, suggesting that residue differences in these segments may affect the folding of hybrid molecules. The 3-D models of the present invention, however, are needed to conduct an amino acid by amino acid analysis of which residues actually directly interact with IgE antibodies.

The FceRIα residues which have been implicated in past studies include residues in the D2 BC loop (amino acid 115), in the C strand (amino acids 117, 118, 120-123), in the C'E loop (amino acids 129, 131), the F strand (amino acids 149, 153) and the FG loop (amino acids 155 and 159) (Cook et al., 1997, *ibid.*; Hulett et al., 1994, *ibid.*; Hulett et al., 1995, *ibid.*). In addition, residues 87 (at the D1D2 interface) and 128 (in the C'E loop) are likely to be part of the IgE interaction site, since mutation of these residues have been shown to influence receptor binding to the IgE point mutant R334A (Cook et al., 1997, *ibid.*). Furthermore, a synthetic peptide corresponding to residues 119-129 has been demonstrated to block IgE binding to the FceRIα, with an apparent K_D of about 3 mM (McDonnell et al., 1997, *ibid.*; McDonnell et al., 1996, *ibid.*).

Analysis of the hFcεRIα model, however, is needed to indicate that of the fifteen residues (i.e., amino acids 87, 115 117, 118, 120-123, 128, 129, 131, 149, 153, 155 and 159), six are buried in the protein core (i.e., amino acids 115, 118, 120, 131, 149, 155)

WO 00/26246 PCT/US99/26203

and predicts that substitution at these positions may lead to indirect structural changes that affect IgE binding. Three of the residues are either partially buried or glycine (i.e., amino acids 122, 129, 153), and substitution may affect the conformation of the local residues. The remaining residues (i.e., amino acids 87, 117, 121, 123, 128, 159) are all exposed amino acids at the FceRIa surface. All of the implicated residues form a contiguous surface extending from the back side of the D2 domain to the top region near the D1D2 interface. Four of the residues are conserved in all human FcRs (i.e., amino acids 87, 118, 149, and 153) and may define a set of common interactions between all FcR receptors and their target Ig molecules.

The hFcεRIα model also indicates that the region of the D2 domain defined by mutagenesis also borders on a number of surface accessible aromatic residues, including four prominent tryptophans at the top of the FcεRIα molecule, namely residues 87, 110, 113, and 156. These four tryptophans form a flat, hydrophobic ridge that neighbors the D2 FG loop. This unusual arrangement of four surface tryptophans probably forms a contact surface for a complementary interaction with an IgE antibody. Tryptophan 87 has already been implicated by mutagenesis studies and tryptophan 156 is prominently displayed at the top of the FG loop. Tryptophan 156 is a glycine in all FcgRs and grafting of residues 154-161 of the FcεRIα FG-loop to FcgRII confers IgE binding. It is to be noted, however, that such a graft does not eliminate IgG binding. The hFcεRIα model predicts that other amino acids, e.g., the tryptophan at residue 87, may be important for antibody class recognition specificity. Other exposed aromatic residues are found concentrated near the IgE binding domain; Fig 6 shows a surface representation of all of the exposed aromatic groups in the hFcεRIα structure, clearly outlining the tryptophan ridge and residues in D2 near the CC'E region.

25 E. Implications for the binding of other FcRs

10

15

20

30

Since carbohydrate would be expected to disrupt any close-packed protein:protein interface, it is interesting to compare the known carbohydrate sites with the proposed IgE-binding site on the receptor surface as defined by models of the present invention. The positions of the carbohydrate attachment sites for seventeen related FcRs indicated that the N-linked carbohydrate sites delineate a boundary around the proposed IgE binding site. This is consistent with the suggestion that related FcRs share a

common binding surface for antibody molecules. Studies of the FcgRII specificity for IgG, for example, have implicated the following residues: amino acids 113-116, 129, 131, 133, 134, 155, 156, and 159-161 (Hulett et al., 1994, *ibid.*; Hulett et al., 1995, *ibid.*). In addition, domain-swap experiments have demonstrated that two of the related FcgRs can form functional hybrid molecules with FceRIa (Hulett et al., 1995, *ibid.*; Mallamaci et al., 1993, *ibid.*), suggesting that these receptors share a common binding surface with their respective antibody ligands. Once again, however, it should be noted that only with the model can one predict exactly which FcR residues directly interact with an Fc domain of an antibody.

The hFceRIa model indicates that the top of the FcR structure is devoid of carbohydrate-attachment sites in the region of D2 that has been implicated in direct interactions with Ig molecules. The neighboring surface of the D1 domain including loops A'B and EF, are also devoid of carbohydrate and could form part of an extended antibody binding site across the D1D2 interface. If these D1 loops are important in determining the specificity and affinity of the FcR:antibody interaction, one might observe sequence variability between high affinity and low IgG receptors and the IgE receptor. This variability in the human IgG and IgE receptors is shown in Fig. 5. For residues 3-173 of the hFceRIa protein, there are 73 amino acid differences that are unique to the IgE receptor as compared to any of the IgG receptors and these are indicated below the sequence alignments. Of these 73 amino acids unique to the human FceRIa protein, 27 positions are highly variable in the different FcR sequences (> 4/7 different amino acids. There are five regions that stand out with clusters of variable residues: residues 27-30, 47-49, 54-33, 94-98 and 155-159. Residues 155-159 (the FG loop) are highly variable and do at least partially determine the specificity of FcR interactions. It is again to be noted that without the model one cannot determine which regions of sequence variability are important in determining FcR protein functional domains.

Previous experiments have shown that residues 27-30 and 47-49 are not critical for FcR specificity (Mallamaci et al., 1993, *ibid.*), and the presence of glycosylation sites within these segments in related FcRs support the suggestion that these regions are not part of the FcR:antibody interaction. The hFccRIα model indicates that residues 94-98

10

15

are found in the A' strand near the D1D2 cleft and therefore are not likely to interact with antibody directly, but these residues might influence interactions indirectly by altering the D1D2 packing interface.

The remaining group of highly variable residues (54-59) are in the D1 E strand (see Fig. 7), near the FcεRIα binding site as predicted by the hFcεRIα model. Residues 54-59 could form a D1 surface of interaction with the Fc domains of antibodies, extending the binding site across both FceRIa domains. This prediction is supported by a study reporting that the exchange of FceRIa residues 55-67 with residues from the FcgRIIIA receptor disrupts the folding of the protein (Mallamaci et al., 1993, ibid.), as some of the residue changes form part of the D1 hydrophobic core. The hFceRIa model also predicts that the neighboring D1 A'B loop (residues 18-21) could also form part of an extended surface of interaction with the antibody. Thus, models of the present invention are needed to interpret data from mutagenesis and swapping experiments.

F. Stoichiometry of binding between FcR and antibody

The activation of FcR-bearing cells requires crosslinking of the receptors, which leads to the activation of intracellular kinase cascades analogous to those in B and T cells. For both high and low high affinity receptors FceRI and FcgRIII, a stoichiometry of 1:1 is observed between the receptor and the Fc domains of the respective antibodies to which they bind (Ghirlando et al., 1995, Biochemistry 34, 13320-13327; Kanellopoulos et al., 1980, ibid.; Keown et al., 1997, Eur. Biophys. J. 25, 471-476), 20 consistent with a requirement for antigen to cause receptor aggregation and activation. The binding site on the Fc domain of an IgE antibody for its receptor has been extensively studied by mutagenesis, implicating amino acids in the third constant domain (Ce3) of the IgE (Basu et al., 1993, J. Biol. Chem. 268, 13118-13127; Henry et al., 1997, Biochemistry 36, 15568-15578; Nissim et al., 1991, Embo J. 10, 101-107; Presta et al., 1994, J. Biol. Chem. 269, 26368-26373). The structure of the Fc domain of IgE antibodies (also referred to as IgE-Fc domains) has not been experimentally determined, but is homologous to the Fc domain of IgG antibodies (also referred to as IgG-Fc domains), for which a number of crystal structures are available (Harris et al., 1998, J. Mol. Biol. 275, 861-872; Huber et al., 1976, Nature 264, 415-420). The 30

residues of the IgE-Fc domain implicated in binding to FceRs based on mutagenesis

analysis are shown mapped onto the structure of the IgG-Fc domain in Fig. 8. The site on an IgG-Fc domain to which FcgRI and FcgRII receptors bind has been mapped to a similar, although smaller, surface that primarily includes residues in the hinge region before the Cg2 domain (Canfield et al., 1991, J. Exp. Med. 173, 1483-1491; Duncan et 5 ...a.., 1988, Nature 332, 563-564; Jefferis et al., 1990, Mol. Immunol. 27, 1237-1240; Lund et al., 1991, J. Immunol. 147, 2657-2662).

An antibody Fc domain is a homodimeric structure that is significantly larger than its respective FcR; see Fig. 8. The observed 1:1 stoichiometry between receptor and antibody indicates that the two-fold symmetry of the Fc domain does not lead to the binding of two FcRs, even with isolated molecules in solution. Without being bound by theory, it is believed that the large and convex nature of the FcR binding surface could span two antibody domains (Cg2 in IgG and Ce3 in IgE) and induce a conformational change in the Fc domain that would prevent the binding of a second FcR to the same antibody. The FcR structure could also form an asymmetric complex with the antibody that sterically blocks the binding of a second FcR, perhaps using the protruding FG loop to block symmetric interactions with the Fc hinge region.

Example 6

20

25

This Example describes the production of additional three-dimensional models of the present invention as well as descriptions of FceRIa proteins predicted therefrom.

A. Production and description of a crystal of PhFc ϵ RI $\alpha_{1.172}$ that belongs to tetragonal space group P4₃, with a=b=145.08Å, c=62.74Å, a=b=g=90°, referred to herein as crystal form T1

Protein PhFceRIa₁₋₁₇₂, having SEQ ID NO:4, was produced using techniques known to those skilled in the art by a lec1 Chinese hamster ovary (CHO) cell line transformed with a nucleic acid molecule encoding the protein, i.e., a nucleic acid molecule comprising SEQ ID NO:3. Crystals were grown in a manner similar to that described in Example 2 via vapor diffusion using a well solution of 20% to 32% PEG 10000, 0.1 M ammonium citrate pH 5.6, and 0.1 M sodium chloride, and a protein starting concentration of 5 to 10 mg/ml. Other size PEGs from 4000 to 20000 were also used, as well as sodium citrate pH 5.6 as a buffer. Other salts such as sodium acetate and ammonium sulfate were also used to grow crystals. The crystal used in the structure

WO 00/26246 PCT/US99/26203

determination, analyzed in a manner similar to that described in Example 4, had five copies of the receptor in the crystallographic asymmetric unit and diffracted to a maximum resolution of 3.1Å. This crystal form, form T1, was refined to a crystallographic R_{free}/R_{work} of 32.78%/29.19% using all the observed data |F| > 0 to 3.1Å and a non-crystallographic symmetry (NCS) restraint constant of 300 kcal/mol Å² for all atoms. There were no waters included in the model. The atomic coordinates of PhFceRIa₁₋₁₇₂, form T1, are listed in Table 5. The solvent accessibilities of the amino acids of PhFceRIa₁₋₁₇₂, form T1, are indicated in Table 9. Table 13 provides crystallographic data and model refinement statistics of PhFceRIa₁₋₁₇₂, form T1. A root mean square (rms) deviation analysis of the alpha carbon positions of PhFcεRIα₁₋₁₇₂, form T1, as compared to PhFceRIa₁₋₁₇₆, form M1, is shown in Table 14. The first line is an overall rms on the segments that align in space. The second two lines are the rms deviations for the loops when the molecules are superimposed according to the first line. Only one copy of model in T1 is compared because the models do not differ by much because of tight NCS restraints.

5

10

15

20

25

В. Production and description of a crystal of PhFceRIa₁₋₁₇₂ that belongs to tetragonal space group P4₃, with a=b=150.50Å, c=74.18Å, α = β = γ =90°, referred to herein as crystal form T2.

Protein PhFceRIa₁₋₁₇₂, having SEQ ID NO:4, was produced using techniques known to those skilled in the art by a lec1 Chinese hamster ovary (CHO) cell line transformed with a nucleic acid molecule encoding the protein, i.e., a nucleic acid molecule comprising SEQ ID NO:3. Crystals were grown and analyzed as described in Example 6A. The crystal used in the structure determination had five copies of the receptor in the crystallographic asymmetric unit and diffracted to a maximum resolution of 3.8Å. This crystal form, form T2, was refined to a crystallographic $R_{\text{free}}/R_{\text{work}}$ of 30.64%/27.99% using all the observed data |F| > 0 to 3.8Å and a NCS restraint constant of 300 kcal/mol $Å^2$ for all atoms. There were no waters included in the model. The atomic coordinates of PhFceRIa₁₋₁₇₂, form T2, are listed in Table 6. The solvent accessibilities of the amino acids of PhFceRI α_{1-172} , form T2, are indicated in Table 10. Table 13 provides crystallographic data and model refinement statistics of PhFcεRIα₁₋₁₇₂,

30

25

30

form T2. A rms deviation analysis of the alpha carbon positions of PhFceRI α_{1-172} , form T2, as compared to PhFceRI α_{1-176} , form M1, is shown in Table 14.

C. Production and description of a crystal of PhFc ϵ RI α_{1-176} that belongs to monoclinic space group C2, with a=136.90Å, b=73.79Å, c=79.40Å, α = γ =90°, and β =117.74°, referred to herein as crystal form M2.

Protein PhFceRIa₁₋₁₇₆, having SEQ ID NO:2, was produced in T. ni Hi-5 cells as described in Example 1. Crystals were grown in a manner similar to that described in Example 2 via vapor diffusion using a well solution of 12% to 20% PEG 4000, 0.1 M HEPES (or Tris) pH 7.5, and 0 to 10% isopropanol, and a protein starting concentration of 5 to 30 mg/ml. The crystal used in the structure determination, analyzed in a manner similar to that described in Example 4, had two copies of the receptor in the crystallographic asymmetric unit and diffracted to a maximum resolution of 3.2Å. This crystal form, form M2, was refined to a crystallographic R_{free}/R_{work} of 28.30%/25.69% using all the observed data |F| > 0 to 3.2Å. A NCS restraint constant of 300 kcal/mol Å² has been imposed for all atoms except certain ones in loops and crystal contacts (residues 1-3, 27-38, 41-43, 69-75, 87, 98, 111-117, 125-135, 144, 152-158 of SEQ ID NO:2) and the N-linked carbohydrate atoms. There were no waters included in the model. The atomic coordinates of PhFceRIa₁₋₁₇₆, form M2, are listed in Table 7. The solvent accessibilities of the amino acids of PhFceRIa₁₋₁₇₆, form M2, are indicated in Table 11. Table 13 provides crystallographic data and model refinement statistics of PhFceRIa₁₋₁₇₆ form M2. A rms deviation analysis of the alpha carbon positions of PhFceRI α_{1-176} , form M2, as compared to PhFceRI α_{1-176} , form M1, is shown in Table 14.

D. Production and description of a crystal of PhFceRI α_{1-172} that belongs to hexagonal space group P6₁22, with a=b=58.62Å, c=229.19Å, α = β = γ =90°, referred to herein as crystal form H1.

Protein PhFceRIa₁₋₁₇₂, having SEQ ID NO:4 except that the isoleucine at position 170 was replaced with cysteine, was produced in a manner similar to that described in Example 1, except that Spodoptera frugiperda Sf9 cells were used instead of T. ni Hi-5 cells. Crystals were grown in a manner similar to that described in Example 2 via vapor diffusion using a well solution of 20% to 30% PEG 4000, 0.1 M sodium citrate pH 5.6,

15

20

25

30

- 0.1 M sodium chloride, and 5-40mM Methyl-6-O-(N-heptylcarbamoyl)-a-D-glucopyranoside (HECAMEG), a protein starting concentration of 10 mg/ml. The crystal used in the structure determination, analyzed in a manner similar to that described in Example 4, had one copy of the receptor in the crystallographic asymmetric unit and diffracted to a maximum resolution of 3.2Å. This crystal form, form H1, was refined to a crystallographic R_{free}/R_{work} of 31.27%/28.78% using all the observed data |F| > 0 to 3.2Å. The atomic coordinates of PhFceRI α_{1-172} , form H1, are listed in Table 8. The solvent accessibilities of the amino acids of PhFceRI α_{1-172} , form H1, are indicated in Table 12. Table 13 provides crystallographic data and model refinement statistics of PhFceRI α_{1-172} , form H1. A rms deviation analysis of the alpha carbon positions of PhFceRI α_{1-172} , form H1, as compared to PhFceRI α_{1-176} , form M1, is shown in Table 14.
- E. The principal differences in the structures from the various crystal forms occurred in the BC loop in domain 1 (the "30 loop"), the C' strand in domain 2 (the "130 region") and the carbohydrate sites. There were also smaller differences in the termini of the structures and the FG loop in domain 1 (the "72 loop").

The 30 loop showed the greatest variability across the different space groups. The density for this loop was often the poorest density in the map, suggesting that the loop may vary in conformation even within a single crystal. In T1 and T2, the density for this loop was higher than the rest (when the molecule was viewed in the normal orientation, with the FG loop of domain 2 at the top and the cleft between the domains at the bottom.) In the tetragonal cells, the 30 loop passed close to residue 51. In the two copies of the receptor in the larger monoclinic cell M2, the 30 loop was pulled down by crystallographic contacts. In these two copies, the density for the 30 loop clearly showed the loop was pulled away from the rest of the molecule to reveal an empty space inside the loop. The location of the 30 loops in H1 and M1 was intermediate to those of the tetragonal cells and M2.

The 130 strand varied across the crystal forms as well. In T1, T2, and the B copy in M2, this strand hydrogen bonded with the C strand in domain 2 to form a canonical C' strand. In the H1 form, the strand crossed over to the other side of the sheet to form a D strand. In the forms M1 and the A copy of M2, this strand was intermediate to a canonical C' and D strand.

WO 00/26246 PCT/US99/26203

-100-

The density at the termini tended to be poorly ordered, but the M2 crystal showed density for the N-terminus. All of the other models began at amino acid 4. The M1 and M2 models were built to residue 174 out of 176 total residues, the H1 model was built to the C-terminal residue 172, and the two tetragonal forms have models that were built to residue 171 out of 172 total residues.

Table 5. Atomic coordinates of PhFceRI α_{1-172} , Form T1

	ATOM	ATOM							
	NUMBER	TYPE	RESIDUE	#	<u> </u>	<u>_Y</u> _	<u></u>	<u>occ</u>	<u> </u>
5	1 2	CB CG	LYS C LYS C	4	14.321	45.864	45.068	1.00	151.11
,	3	CD	LYS C	4	15.396 16.203	44.901 44.418	44.650 45.852	1.00	151.11
	4	CE	LYS C	4	17.285	43.425	45.453	1.00 1.00	151.11 151.11
	5	NZ	LYS C	4	18.066	42.968	46.639	1.00	151.11
10	6	C	LYS C	4	12.828	45.080	43.246	1.00	214.46
10	7 8	0 N	LYS C LYS C	4 4	12.702	44.022	43.863	1.00	214.46
	9	CA	LYS C	4	12.367 13.426	47.226 46.310	44.431 43.920	1.00	214.46
	10	N	PRO C	5	12.448	45.209	41.965	1.00 1.00	214.46 98.70
15	11	CD	PRO C	5	12.271	46.470	41.224	1.00	125.98
15	12 13	CA CB	PRO C	5	11.863	44.086	41.229	1.00	98.70
	14	CG	PRO C PRO C	5 5	10.998 11.793	44.785 45.997	40.181	1.00	125.98
	15	Č	PRO C	5	12.912	43.157	39.866 40.611	1.00 1.00	125.38
	16	0	PRO C	5	14.063	43.545	40.398	1.00	98.70 98.70
20	17	N.	LYS C	6	12.509	41.923	40.330	1.00	208.77
	18 19	CA CB	LYS C	6	13.417	40.948	39.747	1.00	208.77
	20	CG	LYS C LYS C	6 6	14.011 15.074	40.068	40.851	1.00	249.20
	21	CD	LYS C	6	15.769	39.104 38.385	40.363 41.512	1.00 1.00	249.20
25	22	CE	LYS C	6	16.860	37.456	40.986	1.00	249.20 249.20
	23	NZ	LYS C	6	17.633	36.780	42.068	1.00	249.20
	24 25	C O	LYS C	6	12.709	40.087	38.703	1.00	208.77
	26	N	LYS C VAL C	6 7	11.779 13.159	39.341 40.207	39.022	1.00	208.77
30	27	CA	VAL C	7	12.599	40.207 39.454	37.454 36.315	1.00 1.00	73.65 73.65
	28	CB	VAL C	7	13.163	39.923	34.968	1.00	90.39
	29	CG1	VAL C	7	12.395	39.255	33.860	1.00	90.39
	30 31	CG2 C	VAL C VAL C	7	13.095	41.425	34.847	1.00	90.39
35	32	ŏ	VAL C	7 7	12. 87 6 14.017	37.955 37.539	36.338 36.224	1.00	73.65
	33	N	SER C	8	11.833	37.148	36.461	1.00 1.00	73.65 91.19
	34	CA	SER C	8	12.002	35.707	36.469	1.00	91.19
	35	CB	SER C	8	11.113	35.074	37.541	1.00	89.05
40	36 37	OG C	SER C	8 8	9.751	35.407	37.345	1.00	89.05
	38	ŏ	SER C	8	11.625 10.978	35.174 35.870	35.091 34.308	1.00	91.19
	39	N	LEU C	9	12.047	33.946	34.794	1.00 1.00	91.19 76.39
	40	CA	LEU C	9	11.750	33.300	33.511	1.00	76.39
45	41 42	CB	LEU C	9	13.016	33.111	32.687	1.00	48.15
40	43	CG CD1	LEU C	9 9	13.863	34.301	32.245	1.00	48.15
	44	CD2	LEU C	9	14.684 12.964	33.924 35.448	31.048 31.863	1.00 1.00	48.15
	45	Ċ	LEU C	9	11.124	31.922	33.685	1.00	48.1 5 76.39
50	46	0	LEU C	9	11.321	31.262	34.690	1.00	76.39
30	47 48	N CA	ASN C	10	10.380	31.476	32.687	1.00	56.03
	49	CA CB	ASN C ASN C	10 10	9.756	30.161	32.739	1.00	56.03
	50	CG	ASN C	10	8.459 7.912	30.216 28.844	33.531	1.00	97.06
	51	OD1	ASN C	10	8.527	28.844 28.062	33.807 34.532	1.00 1.00	97.06 97.06
55	52	ND2	ASN C	10	6.764	28.528	33.218	1.00	97.06
	53 54	C	ASN C	10	9.460	29.670	31.333	1.00	56.03
	55 55	O N	ASN C PRO C	10 11	8.594 10.173	30.226	30.649	1.00	56.03
	56	CD	PRO C	11	10.173	28.619 28.168	30.873 29.482	1.00	62.47
60	57	CA	PRO C	11	11.225	27.865	31.546	1.00 1.00	141.22 62.47
	58	СВ	PRO C	11	11.726	26.936	30.444	1.00	141.22
	59 60	CG	PRO C	11	10.542	26.774	29.564	1.00	141.22
	61	C	PRO C PRO C	11 11	12.362	28.734	32.097	1.00	62.47
65	62	Ň	PRO C	12	12.512 13.197	29.887 28.186	31.703 33.000	1.00	62.47
	63	CD	PRO C	12	13.127	26.826	33.565	1.00 1.00	68.33 71.60
	64	CA	PRO C	12	14.315	28.913	33.606	1.00	68.33

	65 66	CB CG	PRO C	12 12	· 14.839 13.707	27.958 27.044	34.664 34.925	1.00 1.00	71.60 71.60
	67	C	PRO C	12	15.383	29.190	32.567	1.00	68.33
_	68	. 0	PRO C	12	16.176	30.127	32.696	1.00	68.33
5	69	N	TRP C	13	15.395	28.352	31.538	1.00	58.74
	70 71	CA CB	TRP C	13 13	16.378	28.444	30.466	1.00	58.74
	72	CG	TRP C	13	16.076 15.812	27.401 26.077	29.401 29.969	1.00 1.00	68.19
	73	CD2	TRP C	13	16.476	25.473	31.064	1.00	68.19 68.19
10	74	CE2	TRP C	13	15.848	24.241	31.307	1.00	68.19
	75	CE3	TRP C	13	17.547	25.852	31.873	1.00	68.19
	76 77	CD1 NE1	TRP C	13	14.844	25.220	29.588	1.00	68.19
	77 78	CZ2	TRP C	13 13	14.848 16.252	24.114 23.380	30.391	1.00	68.19
15	79	CZ3	TRP C	13	17.950	23.360 24.993	32.324 32.892	1.00 1.00	68.19
	80	CH2	TRP C	13	17.300	23.771	33.107	1.00	68.19 68.19
	81	С	TRP C	13	16.409	29.810	29.826	1.00	58.74
	82	0	TRP C	13	15.409	30.264	29.288	1.00	58.74
20	83	N CA	ASN C	14	17.570	30.454	29.879	1.00	57.67
20	84 85	CA CB	ASN C ASN C	14 14	17.729	31.775	29.295	1.00	57.67
	86	CG	ASN C	14	18.371 19.809	32.746 32.414	30.304 30.614	1.00	148.07
	87	OD1	ASN C	14	20.127	31.304	31.041	1.00 1.00	148.07
~ "	88	ND2	ASN C	14	20.692	33.383	30.408	1.00	148.07 148.07
25	89	C	ASN C	14	18.508	31.761	27.990	1.00	57.67
	90	0	ASN C	14	18.992	32.785	27.550	1.00	57.67
	91 92	N CA	ARG C	15	18.645	30.590	27.378	1.00	58.44
	93	CB	ARG C ARG C	15 15	19.311 20.634	30.455	26.078	1.00	58.44
30	94	CG	ARG C	15	21.469	29.728 30.131	26.174 27.329	1.00 1.00	68.23
	95	CD	ARG C	15	22.779	29.404	27.261	1.00	68.23 68.23
	96	NE	ARG C	15	23.607	29.885	26.172	1.00	68.23
	97	CZ	ARG C	15	24.492	29.119	25.560	1.00	68.23
35	98	NH1	ARG C	15	24.614	27.865	25.950	1.00	68.23
33	99 100	NH2 C	ARG C ARG C	15	25.267	29.599	24.589	1.00	68.23
	101	ŏ	ARG C	15 15	18.345 18.206	29.540 28.379	25.394 25.805	1.00	58.44
	102	Ň	ILE C	16	17.648	30.048	25.805 24.386	1.00 1.00	58.44 56.07
40	103	CA	ILE C	16	16.691	29.214	23.693	1.00	56.07 56.07
40	104	CB	ILE C	16	15.279	29.668	23.944	1.00	49.05
	105	CG2	ILE C	16	14.939	29.490	25.385	1.00	49.05
	106 107	CG1 CD1	ILE C	16	15.128	31.116	23.520	1.00	49.05
	108	CDI	ILE C	16 16	13.760 16.889	31.675 29.154	23.801	1.00	49.05
45	109	ŏ	ILE C	16	17.607	29.154 29.956	22.201 21.610	1.00 1.00	56.07
	110	N	PHE C	17	16.221	28.178	21.608	1.00	56.07 80.97
	111	CA	PHE C	17	16.247	27.906	20.188	1.00	80.97
	112	CB	PHE C	17	15.846	26.458	19.984	1.00	52.57
50	113	CG	PHE C	17	16.996	25.503	19.972	1.00	52.57
J 0	114 115	CD1 CD2	PHE C	17 17	16.878 18.173	24.248	20.554	1.00	52.57
	116	CE1	PHE C	17	17.897	25.830 23.329	19.278 20.455	1.00	52.57
	117	CE2	PHE C	17	19.207	24.912	19.167	1.00 1.00	52.57 52.57
بر بر	118	CZ	PHE C	17	19.063	23.648	19.759	1.00	52.57
55	119	C	PHE C	17	15.251	28.793	19.468	1.00	80.97
	120	0	PHE C	17	14.320	29.320	20.074	1.00	80.97
	121 122	N CA	LYS C LYS C	18	15.429	28.937	18.161	1.00	59.00
	123	CB	LYS C	18 18	14.529 15.065	29.761 29.846	17.349 15.921	1.00	59.00
60	124	ČĞ	LYS C	18	14.313	30.790	15.003	1.00 1.00	195.91 195.91
	125	CD	LYS C	18	15.142	31.059	13.761	1.00	195.91
	126	CE	LYS C	18	14.441	32.000	12.803	1.00	195.91
	127	NZ	LYS C	18	13.160	31.413	12.321	1.00	195.91
65	128 129	C	LYS C	18	13.123	29.162	17.349	1.00	59.00
J J	130	N	LYS C	18 10	12.937	27.974	17.129	1.00	59.00
	131	CA	GLY C	19 19	12.122 10.774	29.973 29.457	17.630 17.592	1.00	76.33
	132	č	GLY C	19	10.178	28.991	17.582 18.886	1.00 1.00	76.33 76.33
70	133	0	GLY C	19	8.971	28.747	18.970	1.00	76.33 76.33
70	134	N	GLU C	20	10.998	28.857	19.916	1.00	72.26

	405	C 4	0111 0				·		
	135 136	CA CB	GLU C	20	10.460	28.427	21.211	1.00	72.26
	137	CG	GLU C	20 20	11.590 12.410	27.847	22.059	1.00	102.87
	138	CD	GLU C	20	13.457	26.815 26.129	21.296	1.00	102.87
5	139	OE1	GLU C	20	14.291	26.830	22.152 22.758	1.00	102.87
	140	OE2	GLU C	20	13.452	24.884	22.210	1.00 <u>.</u> 1.00	102.87
	141	С	GLU C	20	9.739	29.579	21.956	1.00	102.87 72.26
	142	0	GLU C	20	9.803	30.730	21.525	1.00	72.26 72.26
10	143	N	ASN C	21	9.030	29.264	23.040	1.00	57.87
10	144	CA	ASN C	21	8.336	30.295	23.787	1.00	57.87
	145 146	CB	ASN C	21	6.839	30.041	23.853	1.00	107.77
	147	CG OD1	ASN C ASN C	21	6.273	29.544	22.563	1.00	107.77
	148	ND2	ASN C	21 21	6.639 5.353	30.019 28.591	21.477	1.00	107.77
15	149	C	ASN C	21	8.841	30.401	22.690 25.220	1.00	107.77
	150	Ō	ASN C	21	9.136	29.391	25.859	1.00 1.00	57.87
	151	N	VAL C	22	8.921	31.625	25.735	1.00	57.87 64.18
	152	CA	VAL C	22	9.364	31.858	27.099	1.00	64.18
20	153	CB	VAL C	22	10.797	32.278	27.139	1.00	42.75
20	154 155	CG1	VAL C	22	10.981	33.583	26.376	1.00	42.75
	156	CG2 C	VAL C VAL C	22	11.231	32.452	28.585	1.00	42.75
•	157	ŏ	VAL C	22 22	8.542 8.115	32.997	27.677	1.00	64.18
	158	Ň	THR C	23	8.347	33.897 32.977	26.936 28.998	1.00	64.18
25	159	CA	THR C	23	7.534	33.987	29.693	1.00 1.00	75.81
	160	CB	THR C	23	6.369	33.301	30.399	1.00	75.81 170.16
	161	OG1	THR C	23	5.651	32.492	29.459	1.00	170.16
	162	CG2	THR C	23	5.442	34.327	31.005	1.00	170.16
30	163 164	C	THR C	23	8.328	34.776	30.730	1.00	75.81
50	165	0 N	THR C LEU C	23	8.978	34.183	31.572	1.00	75.81
	166	CA	LEU C	24 24	8.292 9.071	36.101	30.684	1.00	82.13
	167	CB	LEU C	24	9.899	36.861 37.962	31.656 30.995	1.00 1.00	82.13
	168	CG	LEU C	24	10.586	37.719	29.653	1.00	55.82 55.82
35	169	CD1	LEU C	24	11.621	38.790	29.358	1.00	55.82
	170	CD2	LEU C	24	11.241	36.405	29.664	1.00	55.82
	171 172	C	LEU C	24	8.182	37.506	32.677	1.00	82.13
	173	0 N	LEU C THR C	24	7.526	38.505	32.391	1.00	82.13
40	174	CA	THR C	25 25	8.184 7.333	36.967 37.517	33.888	1.00	46.04
	175	CB	THR C	25	6.859	36.406	34.921 35.852	1.00 1.00	46.04
	176	OG1	THR C	25	6.235	35.384	35.064	1.00	88.77 88.77
	177	CG2	THR C	25	5.846	36.939	36.851	1.00	88.77
45	178	Ç	THR C	25	8.047	38.614	35.693	1.00	46.04
43	179 180	0 N	THR C	25	9.225	38.493	36.009	1.00	46.04
	181	CA	CYS C CYS C	26 26	7.360	39.719	35.962	1.00	99.22
٠	182	Č	CYS C	26 26	7.988 7.833	40.779 40.454	36.730	1.00	99.22
	183	ō	CYS C	26	6.787	39.984	38.201 38.644	1.00 1.00	99.22
50	184	СВ	CYS C	26	7.353	42.132	36.440	1.00	99.22 145.11
	185	SG	CYS C	26	8.267	43.513	37.198	1.00	145.11
	186	N	ASN C	27	8.897	40.697	38.944	1.00	197.95
	187	CA	ASN C	27	8.936	40.461	40.370	1.00	197.95
55	188 189	CB CG	ASN C	27	9.427	41.723	41.048	1.00	249.36
55	190	OD1	ASN C ASN C	27	9.841	41.459	42.424	1.00	249.36
	191	ND2	ASN C	27 27	10.558 9.710	40.419 42.399	42. 66 6	1.00	249.36
	192	C	ASN C	27	7.618	40.026	43.346 41.003	1.00 1.00	249.36 197.95
	193	0	ASN C	27	6.829	40.859	41.440	1.00	197.95
60 .	194	N.	GLY C	28	7.392	38.719	41.065	1.00	214.74
	195	CA	GLY C	28	6.162	38.203	41.644	1.00	214.74
	19 6 197	C	GLY C	28	6.121	36.711	41.398	1.00	214.74
	198	N	GLY C ASN C	28	6.177	38.276	40.255	1.00	214.74
65	199	CA	ASN C	29 29	6.006 6.011	35.922	42.456	1.00	249.28
	200	CB	ASN C	29	6.011 6.332	34.476 33.825	42.322 43.676	1.00	249.28
	201	CG	ASN C	29	6.655	32.353	43.576 43.552	1.00 1.00	216.11
	202	OD1	ASN C	29	6.877	31.849	42.450	1.00	216.11 216.11
70	203	ND2	ASN C	29	6.701	31.657	44.681	1.00	216.11
70	204	С	ASN C	29	4.731	33.880	41.751	1.00	249.28

	205 206 207	O N CA	ASN C ASN C ASN C	29 30 30	- 4.781 3.584 2.325	33.119 34.225 33.663	40.788 42.328	1.00 1.00	249.28 235.48
5	208 209	CB CG	ASN C ASN C	30 30	1.763 2.660	32.685 31.487	41.851 42.889 43.106	1.00 1.00 1.00	235.48 219.86
	210 211	OD1 ND2	ASN C ASN C	30 30	3.006 3.040	31.152 30.831	44.240 42.019	1.00	219.86 219.86
	212 213	C	ASN C	30	1.251	34.682	41.498	1.00 1.00	219.86 235.48
10	214	N	PHE C	30 31	0.931 0.690	34.878 35.329	40.325 42.515	1.00 1.00	235.48 241.86
	215 216	CA CB	PHE C	31 31	-0.373 -1.597	36.291 35.920	42.280	1.00	241.86
	217	CG	PHE C	31	-2.076	34.504	43.123 42.908	1.00 1.00	249.47 249.47
15	218 219	CD1 CD2	PHE C PHE C	31 31	-1.432 -3.154	33.431 34.240	43.523 42.066	1.00 1.00	249.47
	220 221	CE1 CE2	PHE C PHE C	31	-1.858	32.115	43.307	1.00	249.47 249.47
	222	CZ	PHE C	31 31	-3.588 -2.936	32.927 31.863	41.843 42.463	1.00 1.00	249.47 249.47
20	223 224	c o	PHE C PHE C	31 31	0.022 0.520	37.743 38.109	42.516 43.587	1.00	241.86
	225 226	N	PHE C	32	-0.212	38.559	41.489	1.00 1.00	241.86 249.62
	226 227	CA CB	PHE C PHE C	32 32	0.108 1.132	39.985 40.302	41.512 40.423	1.00 1.00	249.62 249.66
25	228 229	CG CD1	PHE C PHE C	32 32	1.755 2.582	41.655	40.560	1.00	249.66
	230	CD2	PHE C	32	1.510	41.907 42.675	41.614 39.643	1.00 1.00	249.66 249.66
	231 232	CE1 CE2	PHE C PHE C	32 32	3.147 2.093	43.108 43.918	41.753 39.791	1.00	249.66
30	233 234	cz	PHE C	32	2.900	44.146	40.828	1.00 1.00	249.66 249.66
30	235	CO	PHE C PHE C	32 32	-1.151 -2.197	40.815 40.259	41.269 40.930	1.00 1.00	249.62 249.62
	236 237	N CA	GLU C	33 33	-1.054 -2.224	42.139 42.994	41.416	1.00	249.77
35	238	СВ	GLU C	33	-2.704	43.604	41.200 42.503	1.00 1.00	249.77 249.65
33	239 240	CG CD	GLU C GLU C	33 33	-4.023 -5.159	44.344 43.406	42.358 42.025	1.00 1.00	249.65
	241 242	OE1 OE2	GLU C	33	-5.159	42.298	42.562	1.00	249.65 249.65
40	243	C	GLU C	33 33	-6.051 -2.110	43.779 44.128	41. 23 9 40.194	1.00 1.00	249.65 249.77
40	244 245	0 N	GLU C Val C	33 34	-2.952 -1.107	44.257 44.982	39.301	1.00	249.77
	246	CA	VAL C	34	-0.949	46.113	40.365 39.471	1.00 1.00	243.09 243.09
	247 248	CB CG1	VAL C VAL C	34 34	0.351 0.508	46.880 48.060	39.775 38.826	1.00 1.00	249.25 249.25
45	249 250	CG2	VAL C VAL C	34 34	0.302	47.386	41.184	1.00	249.25
	251	0	VAL C	34	-0.990 -0.603	45.721 44.616	38.002 37.615	1.00 1.00	243.09 243.09
	252 253	N CA	SER C SER C	35 35	-1.494 -1.605	46.644 46.453	37.196	1.00	146.24
50	254 255	CB	SER C	35	-3.021	46.778	35.764 35. 29 0	1.00 1.00	146.24 174.88
	256	OG C	SER C SER C	35 35	-3.296 -0.617	48.166 47.400	35.411 35.103	1.00 1.00	174.83 148.24
	257 258	O N	SER C SER C	35 36	-0.518 0.095	47.438	33.878	1.00	146.21
55	259	CA	SER C	36	1.091	48.179 49.114	35.919 35.408	1.00 1.00	112.51 112.51
	260 261	OG CB	SER C SER C	36 36	0.986 1.420	50.475 50.408	36.105 37.452	1.00	242.80
	262 263	C	SER C	36	2.486	48.535	35.635	1.00 1.00	242.80 112.51
60	264	O N	SER C THR C	36 37	3.088 2.985	48.707 47.834	36.700 34.620	1.00 1.00	112.51 147.41
	265 266	CA CB	THR C THR C	37	4.301	47.220	34.655	1.00	147.41
	267	OG1	THR C	37 37	4.185 3.393	45.679 45.242	34.635 35.748	1.00 1.00	242.04 242.04
65	268 269	CG2 C	THR C THR C	37 37	5.553 5.004	45.039 47.709	34.720	1.00	242.04
-	270	0	THR C	37	4.382	47.708 47.834	33.399 32.345	1.00 1.00	147.41 147.41
	271 272	N CA	LYS C	38 38	6.28 9 7.046	48.009 48.490	33.512 32.361	1.00	114.65
70	273 274	CB	LYS C	38	7.794	49.755	32.733	1.00 1.00	114.65 121.59
, ,	217	CG	LYS C	38	6.890	50.832	33.262	1.00	121.59

277 MZ LYS C 38 7.518 54.413 34.415 1.00 121.59 278 C LYS C 38 38 8.040 46.745 32.852 1.00 114.65 280 N TRP C 39 8.040 46.745 32.852 1.00 114.65 281 CA TRP C 39 8.027 47.373 30.538 1.00 83.37 282 CB TRP C 39 8.027 45.303 30.508 1.00 68.37 283 C C B TRP C 39 8.027 45.303 30.508 1.00 68.37 283 C C B TRP C 39 8.027 45.303 30.508 1.00 68.37 284 C C B TRP C 39 8.027 45.303 30.508 1.00 68.37 285 C C B TRP C 39 8.027 45.303 30.508 1.00 59.20 286 C C B TRP C 39 8.021 42.00 287 C C B TRP C 39 8.021 42.00 288 NE1 TRP C 39 8.021 42.00 31.500 1.00 59.20 288 NE1 TRP C 39 8.021 42.00 31.500 1.00 59.20 280 C C B TRP C 39 7.061 41.892 30.990 1.00 59.20 280 C C TRP C 39 8.021 42.00 31.476 1.00 59.20 280 C C TRP C 39 8.026 44.00 31.476 1.00 59.20 281 C C B TRP C 39 8.026 44.00 31.476 1.00 59.20 282 C C TRP C 39 8.026 44.00 31.476 1.00 59.20 283 N P TRP C 39 8.026 44.00 31.476 1.00 59.20 284 N P TRP C 39 8.026 44.00 31.476 1.00 59.20 285 C C TRP C 39 8.026 44.00 31.476 1.00 59.20 286 C C TRP C 39 8.026 47.779 28.990 1.00 68.37 287 C C B TRP C 39 8.026 47.799 28.990 1.00 68.37 288 N P TRP C 39 8.026 47.799 28.990 1.00 68.37 289 C C TRP C 39 8.026 47.892 29.146 1.00 81.86 286 C C TRP C 39 8.026 47.892 29.144 1.00 83.37 287 C G PHE C 40 12.203 49.801 29.802 20.10 1.00 132.74 288 C C D PHE C 40 11.404 49.258 1.00 13.214 300 C E PHE C 40 11.404 49.258 1.00 13.214 301 C E PHE C 40 11.406 51.803 30.00 1.00 132.74 302 C C PHE C 40 11.406 49.258 30.00 1.00 132.74 303 C C PHE C 40 11.406 51.803 30.00 1.00 132.74 304 C C PHE C 40 11.406 51.803 30.00 1.00 132.74 305 C C R HR C C 40 11.406 44.803 30.00 1.00 132.74 306 C C PHE C 40 11.406 44.803 30.00 1.00 132.74 307 C C C C C C C C C C C C C C C C C C C		275 276	CD CE	LYS C	38 38	· 7.679 6.757	52.074 53.183	33.632 34.088	1.00	121.59
278 C LYS C 38 8 0.045 47.459 31.865 1.00 114.85 280 N TRP C 39 8 0.222 47.373 30.538 1.00 134.85 281 C A TRP C 39 8 0.222 47.373 30.538 1.00 59.20 282 C B TRP C 39 8 0.477 45.308 29.202 1.00 59.20 283 C G TRP C 39 7.651 44.439 30.060 1.00 59.20 284 C D TRP C 39 6.116 43.493 31.026 1.00 59.20 285 C E TRP C 39 6.116 43.493 31.026 1.00 59.20 286 C E TRP C 39 6.116 43.493 31.026 1.00 59.20 287 C E TRP C 39 6.116 43.493 31.00 1.00 59.20 288 C E TRP C 39 6.073 42.881 31.590 1.00 59.20 280 C E TRP C 39 6.073 42.881 31.590 1.00 59.20 281 C E TRP C 39 6.073 42.881 31.590 1.00 59.20 282 C E TRP C 39 6.073 42.881 31.590 1.00 59.20 283 C E TRP C 39 6.073 42.881 43.483 31.00 31.474 1.00 59.20 281 C E TRP C 39 6.073 44.893 30.071 1.00 59.20 281 C E TRP C 39 6.073 44.893 30.071 1.00 59.20 282 C E TRP C 39 8.312 41.694 32.456 1.00 59.20 283 O TRP C 39 8.312 41.594 32.4568 1.00 59.20 283 O TRP C 39 10.086 47.179 32.2488 1.00 68.37 284 N PHE C 40 11.387 46.983 22.144 1.00 88.37 295 C A PHE C 40 11.387 46.983 22.144 1.00 88.37 295 C A PHE C 40 11.387 46.983 29.144 1.00 88.37 295 C A PHE C 40 11.387 46.983 29.144 1.00 88.37 296 C B PHE C 40 11.387 46.983 30.00 12.00 132.74 300 C E PHE C 40 11.387 46.983 30.00 12.00 132.74 300 C E PHE C 40 11.387 46.983 30.00 12.00 132.74 300 C E PHE C 40 11.387 49.591 1.00 132.74 300 C E PHE C 40 11.387 49.591 1.00 132.74 300 C E PHE C 40 11.387 49.288 1.00 13.812 300 C E PHE C 40 11.387 49.288 1.00 13.274 301 ND1 HIS C 41 11.487 49.288 1.00 132.74 302 C E PHE C 40 11.387 49.288 1.00 132.74 303 C E PHE C 40 11.387 49.288 1.00 132.74 304 C E PHE C 40 11.387 49.288 1.00 132.74 305 C E PHE C 40 11.387 49.288 1.00 132.74 307 C B HIS C 41 11.487 49.288 1.00 13.812 308 C G B PHE C 40 11.387 49.288 1.00 13.812 309 C C E PHE C 40 11.387 49.288 1.00 2.288 1.00 13.812 300 C E PHE C 40 11.387 49.288 1.00 2.288 1.00 13.812 300 C E PHE C 40 11.387 49.288 1.00 2.288 1.00 13.812 300 C E PHE C 40 11.487 49.288 1.00 2.288 1.00 13.812 300 C E PHE C 40 11.387 49.288 22.288 1.00 13.812 300 C E PHE C 40 11.487 49.288									1.00	121.59
5 279 O LYS C 38 8.4640 46.745 32.582 1.00 114.882 281 CA TAP C 39 9.182 47.373 30.588 1.00 83.37 282 CB TAP C 39 9.182 46.434 29.954 1.00 83.37 282 CB TAP C 39 7.651 44.439 30.080 1.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00 59.20 10.00	_							_		
280 N TRP C 39 8.222 47.373 30.538 1.00 83.37 281 CA TRP C 39 8.477 45.308 29.202 1.00 59.20 282 CB TRP C 39 8.477 45.308 29.202 1.00 59.20 283 CG TRP C 39 8.477 45.308 30.008 1.00 59.20 284 CB2 TRP C 39 8.477 45.308 31.026 1.00 59.20 285 CB2 TRP C 39 8.318 43.493 31.026 1.00 59.20 287 CB1 TRP C 39 9.391 43.5100 31.474 1.00 59.20 287 CB1 TRP C 39 9.391 43.5100 31.474 1.00 59.20 287 CB1 TRP C 39 5.881 44.393 30.007 1.00 59.20 287 CB1 TRP C 39 5.881 44.393 30.071 1.00 59.20 287 CB1 TRP C 39 5.881 44.393 30.071 1.00 59.20 288 CB2 TRP C 39 5.881 44.393 30.071 1.00 59.20 289 CB2 TRP C 39 5.881 44.393 30.890 1.00 59.20 280 CB3 TRP C 39 5.881 44.393 30.890 1.00 59.20 281 CH2 TRP C 39 5.881 44.393 30.890 1.00 59.20 281 CH2 TRP C 39 5.881 44.393 30.890 1.00 59.20 2821 CH2 TRP C 39 5.881 44.393 30.890 1.00 59.20 283 O TRP C 39 9.912 41.524 29.990 1.00 59.20 284 N PHE C 40 11.387 45.983 29.116 1.00 88.37 285 CA PHE C 40 11.387 45.983 29.116 1.00 88.36 286 CB PHE C 40 11.2300 47.893 29.393 1.00 88.185 286 CB PHE C 40 112.433 49.601 29.952 1.00 132.74 302 CC PHE C 40 11.305 49.601 29.952 1.00 132.74 302 CC PHE C 40 11.305 50.903 29.393 1.00 132.74 302 CC PHE C 40 11.305 50.903 29.393 1.00 132.74 303 CC PHE C 40 11.305 50.903 29.393 1.00 132.74 304 C PHE C 40 11.2433 49.601 29.525 1.00 132.74 305 CB1 PHE C 40 11.2433 49.601 29.525 1.00 132.74 306 CA HIS C 41 11.325 44.667 32.398 29.398 1.00 132.74 307 CB HIS C 41 11.325 44.667 32.398 29.393 1.00 132.74 308 CD1 PHE C 40 11.3264 48.591 29.625 1.00 132.74 309 CB2 PHE C 40 11.3264 48.591 29.525 1.00 132.74 300 CB1 PHE C 40 11.466 49.258 31.056 1.00 132.74 301 CB2 PHE C 40 11.466 49.258 31.056 1.00 132.74 302 CC PHE C 40 11.466 49.258 31.00 13.141 1.00 132.74 303 CB1 PHE C 40 11.466 49.258 31.00 13.141 1.00 132.74 304 CC PHE C 40 11.466 49.258 31.00 13.141 1.00 132.74 305 CC PHE C 40 11.466 49.258 31.00 13.141 1.00 132.74 307 CB HIS C 41 11.437 50.201 31.818 1.00 132.74 308 CD2 PHE C 40 11.467 50.000 50.900 50.900 50.900 50.900 50.900 50.900 50.900 50.900 50.900 50.900 50.900 50.	5				38		46.745			
281 CA TRP C 39 9.182 46.434 29.954 1.00 63.27 282 CG TRP C 39 7.651 44.439 30.060 1.00 59.20 283 CG TRP C 39 7.651 44.439 30.060 1.00 59.20 285 CE2 TRP C 39 6.973 42.881 31.590 1.00 59.20 286 CB3 TRP C 39 8.911 43.100 31.474 1.00 59.20 286 CB3 TRP C 39 8.9191 43.100 31.474 1.00 59.20 286 CB3 TRP C 39 8.9391 43.100 31.474 1.00 59.20 287 CB2 TRP C 39 8.291 43.500 30.071 1.00 59.20 288 REI TRP C 39 8.291 43.500 30.071 1.00 59.20 280 CB3 TRP C 39 7.061 41.892 30.071 1.00 59.20 280 CB3 TRP C 39 8.410 41.892 32.576 1.00 59.20 280 CB3 TRP C 39 8.410 41.892 32.576 1.00 59.20 281 C TRP C 39 8.410 41.892 32.576 1.00 59.20 282 C TRP C 39 8.410 41.892 32.576 1.00 59.20 282 C TRP C 39 8.410 41.892 32.459 1.00 59.20 283 C TRP C 39 8.410 41.892 32.459 1.00 59.20 284 N PHE C 40 11.387 42.113 32.459 1.00 59.20 285 CA PHE C 40 12.330 47.839 28.2484 1.00 59.20 286 CB PHE C 40 11.387 48.593 29.916 1.00 18.37 287 CG PHE C 40 11.387 48.593 29.916 1.00 18.274 297 CG PHE C 40 11.846 49.258 31.653 1.00 132.74 301 CE2 PHE C 40 11.603 51.853 30.100 132.74 301 CE2 PHE C 40 11.603 51.853 30.100 132.74 303 CC1 PHE C 40 11.603 51.853 30.100 132.74 304 C PHE C 40 11.3204 48.591 29.962 1.00 132.74 305 C C PHE C 40 11.327 46.833 49.601 29.852 1.00 132.74 307 C C HE C 40 11.603 51.853 30.130 1.00 132.74 308 C C PHE C 40 11.603 51.853 30.130 1.00 132.74 309 C C PHE C 40 11.603 51.853 30.130 1.00 132.74 301 C C PHE C 40 11.603 51.853 30.130 1.00 132.74 302 C C PHE C 40 11.603 51.853 30.130 1.00 132.74 303 C C PHE C 40 11.603 51.853 30.130 1.00 132.74 304 C PHE C 40 11.603 51.853 30.130 1.00 132.74 305 C C HE C 40 11.603 51.853 30.130 1.00 132.74 307 C C HE C 40 11.603 51.853 30.130 1.00 132.74 308 C C HE C 40 11.603 51.853 30.130 1.00 132.74 309 C C C HE C 40 11.603 51.853 30.130 1.00 132.74 300 C C HE C 40 11.603 51.853 30.130 1.00 132.74 301 C C C HE C 40 11.603 51.853 30.130 1.00 132.74 302 C C PHE C 40 11.603 51.853 30.130 1.00 132.74 303 C C HE C 40 11.603 51.853 30.100 1.00 132.74 304 C C HE C 40 11.603 51.853 30.100 1.00 132.74 305 C C C H						8.222				
282										
10 284 CD2 TRP C 39 7.851 44.439 31.026 1.00 59.20 286 CB2 TRP C 39 6.973 42.881 31.590 1.00 59.20 286 CB2 TRP C 39 6.973 42.881 31.590 1.00 59.20 286 CB2 TRP C 39 9.991 43.100 31.474 1.00 59.20 288 CB2 TRP C 39 9.991 43.100 31.474 1.00 59.20 289 CD2 TRP C 39 7.061 41.882 32.576 1.00 59.20 289 CD2 TRP C 39 7.061 41.882 32.576 1.00 59.20 289 CD2 TRP C 39 7.061 41.882 32.576 1.00 59.20 289 CD2 TRP C 39 8.476 42.119 32.456 1.00 59.20 289 CD2 TRP C 39 8.476 42.119 32.456 1.00 59.20 289 CD2 TRP C 39 8.476 42.119 32.456 1.00 59.20 289 CD2 TRP C 39 8.476 42.119 32.456 1.00 59.20 289 CD2 TRP C 39 8.612 47.779 28.999 1.00 83.37 289 CD2 289 CD2 TRP C 40 11.387 46.983 29.116 1.00 83.37 289 CD2 289 CD2 TRP C 40 11.387 46.983 29.116 1.00 83.37 289 CD2 289 CD2 PHE C 40 11.240 49.891 29.862 1.00 132.74 29.99 CD2 PHE C 40 11.441 50.289 29.852 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.852 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.852 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.892 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.892 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.802 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.892 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.892 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.892 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.892 1.00 132.74 301 CB2 PHE C 40 11.464 49.891 29.892 1.00 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 1.00 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 1.00 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 1.00 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 1.00 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 301 CB2 PHE C 40 11.464 49.893 29.393 3.100 132.74 301 301 CB2 PHE C 40 11.464 49.8										
285 CE2 TFP C 39 9.391 42.881 31.590 1.00 59.20 287 CD1 TFP C 39 9.391 43.100 31.474 1.00 59.20 287 CD1 TFP C 39 6.296 44.369 30.071 1.00 59.20 288 RE1 TFP C 39 6.296 44.369 30.071 1.00 59.20 288 RE1 TFP C 39 7.061 41.892 32.575 1.00 59.20 290 CZ3 TFP C 39 8.312 41.524 32.988 1.00 59.20 291 CH2 TFP C 39 8.312 41.524 32.988 1.00 59.20 292 C TFP C 39 8.312 41.524 32.988 1.00 59.20 293 O TFP C 39 16.12 47.532 28.144 1.00 83.37 293 294 N PHE C 40 11.387 46.963 29.116 1.00 81.36 296 CB PHE C 40 12.330 47.839 28.246 1.00 81.36 296 CB PHE C 40 12.330 47.839 28.246 1.00 81.36 296 CB PHE C 40 12.330 47.839 28.246 1.00 132.74 297 CG PHE C 40 11.446 49.258 31.063 1.00 132.74 300 CE1 PHE C 40 11.346 49.258 31.063 1.00 132.74 300 CE1 PHE C 40 11.305 50.903 29.339 1.00 132.74 300 CE2 PHE C 40 11.00 50.201 31.312 1.00 132.74 300 CE2 PHE C 40 11.00 50.301 29.339 30.10 1.00 132.74 300 CE2 PHE C 40 11.00 50.301 29.339 30.00 132.74 300 CE2 PHE C 40 11.00 50.301 29.339 30.00 132.74 300 CE2 PHE C 40 11.00 50.301 29.339 30.00 132.74 300 CE2 PHE C 40 11.00 50.301 29.339 30.00 132.74 300 CE2 PHE C 40 11.00 50.301 29.339 30.00 132.74 300 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 300 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11.502 51.501 31.344 1.00 132.74 300 CE2 PHE C 40 11	10									59.20
286 CE3 TRP C 39 9.391 43.100 31.474 1.00 59.20 287 CD1 TRP C 39 6.298 44.389 30.071 1.00 59.20 288 NE1 TRP C 39 5.881 43.439 30.990 1.00 59.20 290 CZ2 TRP C 39 7.061 41.892 32.576 1.00 59.20 291 CH2 TRP C 39 9.476 42.119 32.458 1.00 59.20 292 C TRP C 39 10.086 47.179 22.998 1.00 59.20 293 O TRP C 39 10.086 47.179 22.998 1.00 59.20 294 N PHE C 40 11.387 46.963 22.116 1.00 83.37 295 CA PHE C 40 12.300 47.639 22.248 1.00 83.37 296 CB PHE C 40 13.204 48.591 29.062 1.00 81.86 296 CB PHE C 40 13.204 48.591 29.062 1.00 132.74 297 CG PHE C 40 11.387 46.963 22.9116 1.00 81.36 298 CD1 PHE C 40 11.387 46.963 29.116 1.00 81.36 298 CD2 PHE C 40 12.203 47.693 22.248 1.00 81.86 298 CD2 PHE C 40 12.204 48.591 29.062 1.00 132.74 301 CE2 PHE C 40 11.846 49.258 31.063 1.00 132.74 301 CE2 PHE C 40 11.403 51.853 30.100 132.74 301 CE2 PHE C 40 11.003 51.863 30.100 132.74 303 C C PHE C 40 11.020 51.501 31.312 1.00 132.74 303 C C PHE C 40 11.020 51.503 31.010 132.74 303 C C PHE C 40 11.020 51.503 31.010 132.74 303 C C PHE C 40 11.020 51.501 31.312 1.00 132.74 303 C C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C C PHE C 40 11.020 51.501 31.344 1.00 132.74 304 O PHE C 40 14.321 46.333 27.917 1.00 81.86 305 N HIS C 41 13.552 45.334 25.80 1.00 75.89 308 C A HIS C 41 13.552 45.334 25.80 1.00 75.89 311 C B HIS C 41 13.467 46.333 27.917 1.00 81.86 306 C A HIS C 41 14.462 1.00 4.00 70.61 315 N ASN C 42 17.616 46.833 22.393 1.00 75.89 310 ND1 HIS C 41 14.498 45.559 23.528 1.00 75.89 311 C B HIS C 41 14.498 45.559 23.528 1.00 75.89 312 NE2 HIS C 41 14.499 50.646 22.298 20.00 75.89 313 C A SER C 44 11.836 48.922 23.918 1.00 10.51.51 326 C A SER C 44 11.499 50.646 24.2470 1.00 90.93 327 N A SER C 44 11.296 50.666 24.391 1.00 10.51.51 326 C A SER C	10									
287 CD1 TRP C 39 6.298 44.389 30.071 100 59.20 289 CZ2 TRP C 39 7.061 41.892 32.575 1.00 59.20 289 CZ2 TRP C 39 8.476 42.119 32.575 1.00 59.20 289 CZ2 TRP C 39 8.476 42.119 32.545 1.00 59.20 289 CZ2 TRP C 39 8.476 42.119 32.545 1.00 59.20 289 C TRP C 39 8.312 41.524 32.998 1.00 59.20 289 C TRP C 39 8.312 41.524 32.998 1.00 59.20 289 C TRP C 39 9.612 47.932 22.999 1.00 59.20 289 C TRP C 39 9.612 47.932 22.9144 1.00 83.37 289 C C TRP C 40 11.387 46.963 22.116 1.00 83.37 285 CA PHE C 40 12.330 47.839 22.116 1.00 83.37 287 CG PHE C 40 12.330 47.839 22.116 1.00 81.86 289 CD1 PHE C 40 12.330 47.839 12.982 1.00 132.74 300 CE1 PHE C 40 12.305 50.903 29.893 1.00 132.74 300 CE2 PHE C 40 11.805 50.903 29.893 1.00 132.74 301 CE2 PHE C 40 11.805 50.903 29.893 1.00 132.74 303 303 C PHE C 40 11.803 51.853 30.3144 1.00 132.74 304 305 C PHE C 40 11.803 51.853 30.3144 1.00 132.74 305 306 C PHE C 40 11.803 51.853 30.3144 1.00 132.74 307 CB HIS C 41 12.761 46.233 44.759 23.993 1.00 132.74 308 C C PHE C 40 11.803 51.853 30.3144 1.00 132.74 309 300 C PHE C 40 11.803 51.853 30.3144 1.00 132.74 300 304 C PHE C 40 11.803 51.853 30.3144 1.00 132.74 301 CE2 PHE C 40 11.803 51.853 30.3144 1.00 132.74 303 305 N HIS C 41 12.761 46.239 27.9177 1.00 81.86 306 CA HIS C 41 12.761 46.239 23.928 1.00 75.89 307 CB HIS C 41 12.761 46.309 27.9177 1.00 81.86 308 CG HIS C 41 14.4021 46.519 23.928 1.00 75.89 311 CE1 HIS C 41 14.4021 46.519 23.948 1.00 75.89 313 C HIS C 41 14.4021 46.819 23.948 1.00 75.89 313 C HIS C 41 14.4021 46.819 23.948 1.00 75.89 313 C HIS C 41 14.4021 46.819 22.648 1.00 76.61 316 C A SN C 42 17.634 48.807 22.848 1.00 75.89 317 CB ASN C 42 17.649 44.829 23.848 1.00 75.89 318 CD ASN C 42 17.649 44.829 23.848 1.00 75.89 319 CD ASN C 42 17.649 44.829 23.848 1.00 75.89 310 CD ASN C 42 17.649 44.829 23.848 1.00 75.89 311 CEI HIS C 41 14.4021 30.404 31.829 23.848 1.00 75.89 312 C ASN C 42 17.649 48.807 22.849 1.00 70.611 318 CG ASN C 42 17.649 44.807 22.849 1.00 70.015.89 325 C C G C C C C C C C C C C C C C C C C										
15 288 NEI THP C 39 5.881 43.435 30.990 1.00 59.20 290 CZ2 TRP C 39 7.061 41.892 23.2578 1.00 59.20 291 CH2 TRP C 39 8.476 42.119 22.456 1.00 59.20 291 CH2 TRP C 39 8.476 42.119 22.456 1.00 59.20 291 CH2 TRP C 39 8.112 41.524 32.998 1.00 59.20 292 C TRP C 39 8.112 41.524 32.998 1.00 59.20 293 O TRP C 39 8.112 41.524 32.998 1.00 59.20 294 N PHE C 40 11.387 46.963 22.116 1.00 83.37 295 CR PHE C 40 11.387 46.963 22.116 1.00 83.37 295 CR PHE C 40 12.300 47.639 22.248 1.00 81.86 296 CR PHE C 40 13.204 48.591 29.062 1.00 132.74 297 CG PHE C 40 13.204 48.591 29.062 1.00 132.74 298 CD PHE C 40 11.846 49.258 31.063 1.00 132.74 298 CD PHE C 40 11.846 49.258 31.063 1.00 132.74 298 CD PHE C 40 11.846 49.258 31.063 1.00 132.74 298 CD PHE C 40 11.603 51.853 30.100 132.74 298 CD PHE C 40 11.003 51.853 30.100 132.74 301 CE2 PHE C 40 11.003 51.853 30.100 10.00 132.74 301 CE2 PHE C 40 11.003 51.853 30.100 132.74 301 CE2 PHE C 40 11.003 51.853 30.100 10.00 132.74 302 CZ PHE C 40 11.003 51.853 30.100 10.00 132.74 303 303 C PHE C 40 11.003 51.853 30.100 10.00 132.74 303 303 C PHE C 40 11.003 51.853 30.100 10.00 132.74 303 303 C PHE C 40 11.003 51.853 30.100 10.00 132.74 303 303 C PHE C 40 11.003 51.853 30.100 10.00 132.74 303 303 C PHE C 40 11.003 51.853 30.100 10.00 132.74 303 303 C PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 307 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 308 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 308 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 308 CB PHE C 40 11.003 51.853 30.100 10.00 70.81 308 CB PHE C 40 11.003 51.853 30.100 70.81 308 50 CB PHE C 40 11.003 51.853 30.100 70.81 30.00 70.81 30.00 70.81 30.00 70.81 30.00 7										
15 289 CZ2 TRP C 39 7.061 41.892 32.576 1.00 55.20 290 CZ3 TRP C 39 8.476 42.119 32.456 1.00 55.20 291 CH2 TRP C 39 8.376 42.119 32.456 1.00 55.20 292 C TRP C 39 8.312 41.524 32.998 1.00 55.20 292 C TRP C 39 10.086 471.779 28.990 1.00 83.37 292 293 O TRP C 39 10.086 471.779 28.990 1.00 83.37 295 CA PHE C 40 11.387 46.963 29.116 1.00 81.86 296 CB PHE C 40 12.330 47.639 28.248 1.00 81.86 296 CB PHE C 40 12.330 47.639 28.248 1.00 81.86 296 CB PHE C 40 12.330 47.639 28.248 1.00 132.74 299 CD2 PHE C 40 12.433 49.501 29.552 1.00 132.74 300 CE1 PHE C 40 11.846 49.558 31.063 1.00 132.74 300 CE1 PHE C 40 11.441 50.201 31.01 32.74 300 CE1 PHE C 40 11.603 57.853 30.130 1.00 132.74 300 CE2 PHE C 40 11.020 57.503 30.30 1.00 132.74 300 CE2 PHE C 40 11.020 57.503 30.30 1.00 132.74 300 CE2 PHE C 40 11.020 57.503 30.30 1.00 132.74 300 CE2 PHE C 40 11.020 57.503 30.30 1.00 132.74 300 CE2 PHE C 40 11.5225 46.677 37.7474 1.00 132.74 300 CE2 PHE C 40 11.020 57.503 30.30 1.00 132.74 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 132.74 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 132.74 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 132.74 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 132.74 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 132.74 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 132.74 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 70.61 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 70.61 300 CE3 PHE C 40 11.5225 46.677 37.7474 1.00 70.61 300 CE3 PHE C 40 11.5252 46.677 37.7474 1.00 70.61 300 CE3 PHE C 40 11.5252 46.677 37.7474 1.00 70.61 300 CE3 PHE C 40 11.3225 44.671 37.500 PHE C 40 11.5252 46.677 37.7474 1.00 70.61 300 PHE C 40 11.3225 44.671 30.00 PHE C 40 11.00 PHE C 40 11.3225 44.671 30.00 PHE C 40 11.3225 44.671 30.00 PHE C 40 11.		288								
290 CZ3 TRP C 39 9.476 42.119 32.456 1.00 59.20 291 CH2 TRP C 39 48.312 41.524 32.998 1.00 59.20 292 C TRP C 39 10.086 47.179 28.990 1.00 83.37 20 294 N PHE C 40 11.387 46.963 29.116 1.00 83.37 295 CA PHE C 40 11.387 46.963 29.116 1.00 83.37 295 CA PHE C 40 11.3204 48.591 29.062 1.00 132.74 296 CB PHE C 40 12.330 47.659 29.652 1.00 132.74 297 CG PHE C 40 11.2433 49.501 29.852 1.00 132.74 298 CD1 PHE C 40 11.846 49.258 31.063 1.00 132.74 300 CE1 PHE C 40 11.846 49.258 31.063 1.00 132.74 301 CE2 PHE C 40 11.411 50.201 31.314 1.00 132.74 301 CE2 PHE C 40 11.205 50.903 29.393 1.00 132.74 302 CZ PHE C 40 11.205 51.501 31.314 1.00 132.74 303 CC CZ PHE C 40 11.225 46.677 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.677 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.677 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.577 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.577 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.577 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.577 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.577 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.577 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 46.577 27.474 1.00 132.74 303 CC CZ PHE C 40 11.225 42.25 40.07 0.00 70.61 307 CC R HIS C 41 11.253 43.501 29.25 10.00 70.61 307 CC R HIS C 41 11.253 43.501 29.25 10.00 70.61 307 CC R HIS C 41 11.4527 42.893 22.314 1.00 70.61 307 CC R HIS C 41 11.4527 42.893 22.318 1.00 75.99 310 ND1 HIS C 41 11.409 42.297 22.892 1.00 75.99 312 NES C 40 11.427 42.893 22.393 1.00 75.99 312 NES C 40 11.427 42.893 22.393 1.00 75.99 312 NES C 41 11.4327 42.893 22.393 1.00 75.99 312 NES C 41 11.4327 42.893 22.393 1.00 0.093 312 NES C 41 11.4327 42.893 22.393 1.00 0.093 312 NES C 41 11.4327 42.893 22.393 1.00 0.093 312 NES C 41 11.4327 42.893 22.393 1.00 0.00 75.99 312 NES C 41 11.4327 42.893 22.393 1.00 0.00 75.99 312 NES C 41 11.4327 42.893 22.393 1.00 0.00 75.99 312 NES C 41 11.4327 42.893 22.393 1.00 0.00 75.99 312 NES C 41 11.4327 42.893 22.393 1.00 0.00 95.93 312 NES C 41 11.4327 32.306 32.30 NES C 42 11.44329 32.30	15	289		TRP C			41.892			
291 CH2 TRP C 39 8.312 41.524 32.998 1.00 59.20 292 C TRP C 39 10.096 47.179 28.990 1.00 83.37 20 293 O TRP C 39 9.612 47.532 28.144 1.00 83.37 20 294 N PHE C 40 11.387 46.963 29.116 1.00 91.86 295 CA PHE C 40 12.330 47.639 28.248 1.00 81.86 296 CB PHE C 40 12.330 47.639 28.248 1.00 181.86 297 CG PHE C 40 12.330 49.601 29.552 1.00 132.74 298 CD1 PHE C 40 12.333 49.601 29.552 1.00 132.74 300 CE1 PHE C 40 11.846 49.258 31.063 1.00 132.74 301 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 302 CZ PHE C 40 11.020 51.501 31.812 1.00 132.74 303 CC PHE C 40 11.020 51.501 31.812 1.00 132.74 304 305 C PHE C 40 11.020 51.501 31.344 1.00 132.74 305 N HIS C 41 12.255 45.334 25.490 1.00 70.61 306 CA HIS C 41 13.552 45.334 25.490 1.00 70.61 307 CB HIS C 41 13.552 45.334 25.490 1.00 70.61 308 CG HIS C 41 14.327 42.893 29.333 1.00 75.89 310 ND1 HIS C 41 14.327 42.893 29.333 1.00 75.89 311 CE1 HIS C 41 14.676 42.297 22.892 1.00 75.89 312 NEZ HIS C 41 14.676 44.692 29.918 1.00 75.89 313 ND1 HIS C 41 14.676 44.692 29.918 1.00 75.89 312 NEZ HIS C 41 14.671 46.18 24.794 1.00 70.61 315 N ASN C 42 17.063 46.600 24.515 1.00 90.93 316 CA ASN C 42 17.169 44.897 22.991 1.00 70.61 316 CA ASN C 42 17.169 44.892 29.918 1.00 75.89 317 CB ASN C 42 17.169 44.893 22.991 1.00 70.61 316 CA ASN C 42 17.169 44.893 22.991 1.00 70.61 317 CB ASN C 42 17.169 44.893 22.991 1.00 70.61 316 CA ASN C 42 17.169 44.893 22.991 1.00 76.89 317 CB ASN C 42 17.169 44.893 22.991 1.00 90.99 318 CG ASN C 42 17.691 44.896 48.077 22.991 1.00 90.99 319 CD ASN C 42 17.693 44.690 22.291 1.00 90.99 320 CD ASN C 42 17.693 44.690 22.291 1.00 90.93 310 ND1 ASN C 42 17.693 44.690 22.291 1.00 90.99 320 CD ASN C 42 17.693 46.690 24.615 1.00 90.93 321 C HIS C 44 11.496 50.164 50.07 22.997 1.00 10.51 326 C GLY C 43 16.976 50.902 22.997 1.00 10.51 327 N SER C 44 11.492 50.140 24.769 1.00 1.51 328 C A ASN C 42 17.693 46.690 24.615 1.00 90.93 329 C D SER C 44 11.886 48.992 22.909 1.00 11.51 326 C G GLY C 43 16.976 50.902 22.502 1.00 11.51 327 N SER C 44 11.886 48.992 22.705 1.00 11.52					39					
292 CC								32.998		
200 294 N PHE C 40 11.387 46.983 29.116 1.00 81.86 296 CB PHE C 40 12.303 47.839 28.248 1.00 81.86 296 CB PHE C 40 13.204 47.839 28.248 1.00 132.74 298 CD1 PHE C 40 12.433 49.601 29.852 1.00 132.74 300 CE1 PHE C 40 12.433 49.601 29.852 1.00 132.74 300 CE1 PHE C 40 11.846 49.258 31.063 1.00 132.74 300 CE1 PHE C 40 11.846 49.258 31.063 1.00 132.74 300 CE1 PHE C 40 11.603 51.853 30.130 1.00 132.74 300 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 300 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 300 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 300 CE2 PHE C 40 13.225 46.677 27.474 1.00 132.76 303 CC PHE C 40 13.225 46.677 27.474 1.00 81.86 306 CA HIS C 41 13.552 46.677 27.474 1.00 81.86 306 CA HIS C 41 13.552 45.334 25.490 1.00 70.61 307 CB HIS C 41 13.552 45.334 25.490 1.00 70.81 308 CG HIS C 41 13.552 43.554 25.390 28.514 1.00 70.81 307 CB HIS C 41 13.259 43.559 23.528 1.00 75.89 310 ND1 HIS C 41 14.227 42.893 23.528 1.00 75.89 311 CE1 HIS C 41 14.093 42.898 21.826 1.00 75.89 311 CE1 HIS C 41 14.093 42.898 21.826 1.00 75.89 311 CE1 HIS C 41 14.093 42.898 21.826 1.00 75.89 311 CE1 HIS C 41 14.093 42.898 21.826 1.00 75.89 311 CE1 HIS C 41 14.697 42.893 23.918 1.00 75.89 311 CE1 HIS C 41 14.697 42.893 23.918 1.00 75.89 311 CE1 HIS C 41 14.697 42.893 23.918 1.00 75.89 311 CE1 HIS C 41 14.697 42.893 23.918 1.00 75.89 311 CE1 HIS C 41 14.697 42.893 23.898 21.826 1.00 75.89 311 CE1 HIS C 41 14.697 42.893 23.898 21.826 1.00 75.89 311 CE1 HIS C 41 14.492 42.897 23.898 21.826 1.00 75.89 311 CE1 HIS C 41 14.492 42.897 22.898 21.00 75.89 311 CE1 HIS C 41 14.492 42.897 22.898 21.00 75.89 311 CE1 HIS C 41 14.492 42.897 22.898 21.00 75.89 311 CE1 HIS C 41 14.492 42.897 22.898 21.00 75.89 311 CE1 HIS C 41 14.492 42.897 22.898 21.00 75.89 311 CE1 HIS C 41 14.492 42.897 22.898 21.806 1.00 10.51 312 42.898 312 C 3.898										
295 CA PHE C 40 12.330 47.839 28.248 1.00 81.86 296 CB PHE C 40 13.204 48.591 29.062 1.00 132.74 297 CG PHE C 40 13.204 48.591 29.062 1.00 132.74 300 CD2 PHE C 40 11.846 49.258 31.063 1.00 132.74 301 CE2 PHE C 40 11.041 50.201 31.812 1.00 132.74 301 CE2 PHE C 40 11.020 51.851 30.130 1.00 132.74 302 CZ PHE C 40 11.020 51.851 30.130 1.00 132.74 303 C PHE C 40 11.020 51.851 30.130 1.00 132.74 303 C C PHE C 40 11.020 51.851 30.130 1.00 132.74 303 C C PHE C 40 11.020 51.851 30.130 1.00 132.74 305 N HIS C 41 12.761 46.333 27.917 1.00 81.86 306 N HIS C 41 13.275 46.333 27.917 1.00 81.86 307 CB HIS C 41 13.552 45.334 22.5114 1.00 70.61 307 CB HIS C 41 13.399 43.567 22.198 1.00 75.99 310 ND1 HIS C 41 14.327 42.893 23.328 1.00 75.99 311 ND1 HIS C 41 14.765 42.207 22.892 1.00 75.99 312 NE2 HIS C 41 14.765 42.207 22.892 1.00 75.99 312 NE2 HIS C 41 14.765 42.207 22.892 1.00 75.99 313 C HIS C 41 14.765 42.207 22.892 1.00 75.99 314 O HIS C 41 14.693 42.598 21.326 1.00 75.99 315 N ASN C 42 17.150 46.632 23.918 1.00 75.99 316 CA ASN C 42 17.150 46.603 23.933 1.00 75.99 317 CB ASN C 42 17.150 46.403 23.903 1.00 75.99 318 CG ASN C 42 17.150 46.403 23.983 1.00 75.99 319 ND1 ASN C 42 17.160 46.403 23.983 1.00 75.99 310 ND1 HIS C 41 14.093 42.598 21.326 1.00 75.99 311 CEI HIS C 41 14.093 42.598 21.326 1.00 75.99 312 NE2 HIS C 41 14.693 42.598 21.326 1.00 75.99 313 C HIS C 41 14.693 42.598 21.326 1.00 75.99 314 O HIS C 41 14.693 42.598 21.326 1.00 75.99 315 N ASN C 42 17.150 46.403 23.983 1.00 75.99 316 CA ASN C 42 17.150 46.403 23.983 1.00 75.99 317 CB ASN C 42 17.150 46.403 22.3918 1.00 70.61 318 CG ASN C 42 17.161 45.987 22.641 1.00 90.93 319 CD ASN C 42 17.160 46.403 23.985 1.00 90.93 321 C ASN C 42 17.160 46.403 23.985 1.00 90.93 322 O ASN C 42 17.160 46.403 22.251 1.00 101.51 325 C G GLY C 43 14.295 50.466 52.997 1.00 101.51 326 C G GLY C 43 14.295 50.466 52.997 1.00 101.51 327 N SER C 44 13.276 50.466 50.997 1.00 158.29 329 CB SER C 44 13.276 50.466 25.997 1.00 101.51 326 C G GLY C 45 7.785 50.602 22.551 1.00 19.898 323 O G G	20									83.37
296 CB PHE C 40 13.204 48.591 29.062 1.00 132.74 298 CD1 PHE C 40 11.846 49.258 31.063 1.00 132.74 300 CE1 PHE C 40 11.846 49.258 31.063 1.00 132.74 300 CE1 PHE C 40 11.846 49.258 31.063 1.00 132.74 301 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 302 CZ PHE C 40 11.603 51.853 30.130 1.00 132.74 303 CC PHE C 40 11.620 51.851 30.130 1.00 132.74 303 CC PHE C 40 11.620 51.851 30.100 70.811 303 CC PHE C 40 13.225 46.677 27.474 1.00 81.86 306 CA HIS C 41 12.761 46.239 26.314 1.00 70.61 307 CB HIS C 41 12.633 44.671 24.470 1.00 75.89 308 CG HIS C 41 13.552 45.334 25.480 1.00 75.89 310 ND1 HIS C 41 13.192 43.557 22.188 1.00 75.89 311 ND1 HIS C 41 14.765 42.287 22.882 1.00 75.89 311 ND1 HIS C 41 14.765 42.287 22.882 1.00 75.89 312 NEZ HIS C 41 11.4093 42.598 21.826 1.00 70.61 313 C HIS C 41 14.4093 42.598 21.826 1.00 75.89 313 C HIS C 41 14.4093 42.598 21.826 1.00 75.89 313 C HIS C 41 14.693 42.598 21.826 1.00 75.89 313 C HIS C 41 14.4093 42.598 21.826 1.00 75.89 313 C HIS C 41 14.4093 42.598 21.826 1.00 75.89 313 C HIS C 41 14.4093 42.598 21.826 1.00 75.89 313 C HIS C 41 14.4093 42.598 21.826 1.00 75.89 313 C HIS C 41 14.4093 42.598 21.826 1.00 75.89 315 N ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.613 45.807 22.641 1.00 90.99 317 CB ASN C 42 17.159 46.463 23.3085 1.00 90.99 317 CB ASN C 42 17.614 45.807 22.641 1.00 90.93 322 O ASN C 42 17.615 45.807 22.641 1.00 90.93 323 N GLY C 43 14.295 50.466 22.23 1.00 101.51 325 C ASN C 42 17.614 45.907 22.641 1.00 90.93 321 C ASN C 42 17.615 45.916 45.977 1.00 101.51 325 C ASN C 42 17.616 45.917 1.00 101.51 326 C ASN C 42 17.619 45.917 1.00 101.51 327 N SEP C 44 11.489 50.460 24.265 1.00 101.51 328 CA ASN C 42 17.619 49.907 22.641 1.00 101.51 326 C ASN C 42 17.619 49.907 22.641 1.00 101.51 327 N SEP C 44 11.886 49.802 22.318 1.00 101.51 328 CA SEP C 44 11.886 49.802 22.318 1.00 101.51 329 C ASN C 42 16.966 49.707 22.641 1.00 101.51 329 C ASN C 42 16.966 49.707 22.641 1.00 101.51 329 C ASR C 44 11.886 49.802 22.705 1.00 101.51 329 C ASR C 44 11.886 49.805 24.00	20									
297 CG PHE C 40 12.433 49.601 29.852 1.00 132.74 298 CD1 PHE C 40 11.846 49.258 31.063 1.00 132.74 301 CE2 PHE C 40 11.141 50.201 31.812 1.00 132.74 301 CE2 PHE C 40 11.020 51.851 30.130 1.00 132.74 302 CZ PHE C 40 11.020 51.851 30.130 1.00 132.74 303 C PHE C 40 11.020 51.851 30.130 1.00 132.74 303 C PHE C 40 11.020 51.851 30.130 1.00 132.74 303 C PHE C 40 11.020 51.851 30.130 1.00 132.74 303 C PHE C 40 13.225 46.677 27.474 1.00 81.86 305 N HIS C 41 12.761 46.239 28.314 1.00 70.81 306 CA HIS C 41 12.633 44.671 307 CB HIS C 41 12.633 43.759 23.528 1.00 75.99 310 ND1 HIS C 41 13.339 43.759 23.528 1.00 75.99 310 ND1 HIS C 41 14.327 42.883 23.833 1.00 75.99 311 NE2 HIS C 41 14.765 42.207 22.882 1.00 75.99 312 NE2 HIS C 41 14.693 42.896 21.826 1.00 75.99 313 C HIS C 41 14.693 42.998 21.826 1.00 75.99 314 O HIS C 41 14.693 42.998 21.826 1.00 75.99 315 N ASN C 42 17.150 46.403 23.983 1.00 75.99 316 CA ASN C 42 17.169 46.802 23.918 1.00 75.99 317 CB ASN C 42 17.169 46.803 23.905 1.00 90.99 318 CG ASN C 42 17.169 46.803 23.983 1.00 90.93 319 ND2 ASN C 42 17.169 46.803 23.983 1.00 90.93 310 ND2 ASN C 42 17.169 46.803 23.983 1.00 90.93 311 CB ASN C 42 17.169 46.803 23.983 1.00 90.93 312 NE2 HIS C 41 14.4093 42.998 21.826 1.00 75.99 318 CG ASN C 42 17.169 46.803 23.983 1.00 90.93 319 ND2 ASN C 42 17.169 46.803 23.983 1.00 90.93 310 ND2 ASN C 42 17.169 46.803 23.983 1.00 90.93 317 CB ASN C 42 17.169 46.803 23.983 1.00 90.93 318 CG ASN C 42 17.169 44.807 22.841 1.00 90.93 319 ND2 ASN C 42 18.405 45.077 21.649 1.00 90.93 320 ND2 ASN C 42 17.169 44.805 25.206 1.00 101.51 325 C GLY C 43 16.96 45.077 24.891 1.00 101.51 326 C ASN C 42 17.606 46.803 23.985 1.00 101.51 327 N SER C 44 11.806 50.866 24.815 1.00 19.83 320 ND2 ASN C 42 18.405 50.866 24.812 1.00 158.89 321 C ASS C 44 11.806 50.866 24.812 1.00 158.89 322 N GLY C 43 16.966 45.907 1.00 158.29 323 N GLY C 43 16.966 45.907 22.856 1.00 101.51 326 C GLY C 43 16.966 45.907 22.856 1.00 158.29 327 N SER C 44 11.806 50.866 24.812 1.00 158.89 329 CB SER C 44 11.866 45.907 22.856 1.										
25 289 CD1 PHE C 40 11,846 49.258 31.063 1.00 132,74 300 CE1 PHE C 40 11.0305 50.903 29.393 1.00 132,74 301 CE2 PHE C 40 11.030 51.853 30.130 1.00 132,74 302 CZ PHE C 40 11.020 51.501 31.341 1.00 132,74 303 303 C PHE C 40 11.020 51.501 31.344 1.00 132,74 303 304 O PHE C 40 13.225 46.677 27,474 1.00 81.86 305 N HIS C 41 12,761 46.239 28.314 1.00 71.861 306 CA HIS C 41 12,761 46.239 28.314 1.00 71.861 307 CB HIS C 41 13.552 45.334 25.490 1.00 770.61 308 CG HIS C 41 13.539 43,759 23.528 1.00 75.99 311 CE1 HIS C 41 14.327 42.883 23.933 1.00 75.99 311 CE1 HIS C 41 14.032 42.883 23.933 1.00 75.99 311 CE1 HIS C 41 14.032 42.883 23.933 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.671 46.118 24.794 1.00 70.61 316 CA ASN C 42 17.150 46.483 22.9318 1.00 75.99 317 CB ASN C 42 17.150 46.483 22.9318 1.00 75.99 318 CG ASN C 42 17.150 46.483 22.9318 1.00 70.61 316 CA ASN C 42 17.150 46.483 23.983 1.00 90.93 317 CB ASN C 42 17.150 46.483 23.983 1.00 90.93 318 CG ASN C 42 17.150 46.483 23.085 1.00 90.93 319 CD ASN C 42 17.150 46.483 23.085 1.00 90.93 310 C ASN C 42 17.150 46.483 23.085 1.00 90.93 311 CE HIS C 41 14.476 45.877 25.884 1.00 90.93 312 NB CG ASN C 42 17.150 46.483 23.085 1.00 90.93 313 C C BSS C 44 11.4761 45.087 25.186 1.00 90.93 316 CA ASN C 42 17.150 46.483 23.085 1.00 90.93 317 CB ASN C 42 17.150 46.483 23.085 1.00 90.93 320 ND2 ASN C 42 17.150 46.483 23.085 1.00 90.93 321 C ASN C 42 17.150 46.483 23.085 1.00 90.93 322 O ASN C 42 17.150 46.483 23.085 1.00 90.93 323 N GLY C 43 18.315 43.394 25.997 1.00 101.51 326 C G GLY C 43 16.966 48.077 24.971 1.00 90.93 321 C SER C 44 13.183 50.282 25.114 1.00 19.88 322 O ASN C 42 17.617 49.792 26.478 1.00 101.51 326 C G GLY C 43 16.375 50.612 22.007 1.00 101.51 327 N SER C 44 11.886 48.982 25.114 1.00 159.89 329 CB SER C 44 13.183 50.282 25.056 1.00 11.327 338 CD2 LEU C 45 9.126 49.705 25.661 1.00 11.327 338 CD2 LEU C 45 9.126 49.705 25.661 1.00 11.327 339 CD1 LEU C 45 9.126 49.705 25.661 1.00 11.00 127.30 344 CD SER C 46 8.848 48.788 45.788 2										
25) 299 CD2 PHE C 40 12.305 50.903 29.393 1.00 132.74 300 CE1 PHE C 40 11.01 50.201 31.812 1.00 132.74 301 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 302 CZ PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C PHE C 40 11.020 51.501 31.344 1.00 132.74 303 C PHE C 40 13.225 46.677 27.474 1.00 81.86 305 N HIS C 41 12.761 46.239 28.314 1.00 70.61 306 CA HIS C 41 13.552 45.334 25.490 1.00 70.61 307 CB HIS C 41 13.552 45.334 25.490 1.00 70.61 308 CG HIS C 41 13.339 43.759 23.528 1.00 75.99 310 ND1 HIS C 41 13.192 43.567 22.198 1.00 75.99 310 ND1 HIS C 41 14.327 42.893 1.00 75.99 311 CE1 HIS C 41 14.766 42.207 22.892 1.00 75.99 312 NE2 HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C C HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C C HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C C HIS C 41 14.693 42.599 21.528 1.00 70.61 315 N ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.160 44.482 20.95 23.918 1.00 70.61 316 CA ASN C 42 17.163 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.163 46.600 24.615 1.00 90.93 320 ND2 ASN C 42 17.474 48.926 48.077 24.971 1.00 90.93 321 C ASN C 42 17.474 48.926 48.077 24.971 1.00 90.93 322 O ASN C 42 17.474 48.926 48.077 24.971 1.00 90.93 323 N GLY C 43 16.315 48.994 26.086 1.00 10.51 326 C ASN C 42 17.474 48.926 22.267 1.00 10.51 327 N SER C 44 11.886 48.902 25.114 1.00 19.53 328 CA EE C 44 11.886 48.902 25.114 1.00 19.53 329 CB SER C 44 11.886 48.902 25.114 1.00 19.53 330 CD LEU C 45 7.855 51.691 27.238 1.00 113.27 333 C SER C 44 11.886 48.902 25.114 1.00 19.53 334 CA LEU C 45 9.909 50.882 26.091 1.00 19.53 336 CB LEU C 45 7.855 51.691 27.238 1.00 113.27 336 CB LEU C 45 7.855 51.691 27.238 1.00 113.27 337 CD1 LEU C 45 9.909 50.882 26.091 1.00 19.53 344 CA SER C 46 8.458 48.758 25.915 1.00 110.459										
300 CE1 PHE C 40 11.141 50.201 31.812 1.00 132.74 301 CE2 PHE C 40 11.603 51.853 30.130 1.00 132.74 302 CZ PHE C 40 11.602 51.501 31.344 1.00 132.74 303 C PHE C 40 11.202 51.501 31.344 1.00 132.74 303 304 O PHE C 40 13.225 48.677 27.474 1.00 81.86 305 N HIS C 41 12.761 46.239 26.314 1.00 70.61 306 CA HIS C 41 12.761 46.239 26.314 1.00 70.61 307 CB HIS C 41 12.633 44.671 24.470 1.00 75.99 308 CG HIS C 41 13.339 43.759 23.528 1.00 75.99 309 CD2 HIS C 41 13.192 43.567 22.198 1.00 75.99 310 ND1 HIS C 41 14.023 42.598 21.826 1.00 75.99 311 CE1 HIS C 41 14.023 42.598 21.826 1.00 75.99 312 NE2 HIS C 41 14.003 42.598 21.826 1.00 75.99 313 C HIS C 41 14.671 46.118 24.774 1.00 70.61 315 N ASN C 42 17.063 46.600 24.615 1.00 70.61 316 CA ASN C 42 17.163 46.600 24.615 1.00 90.93 317 CB ASN C 42 17.163 46.600 24.615 1.00 90.93 318 CG ASN C 42 17.163 46.600 24.615 1.00 90.93 319 OD1 ASN C 42 17.161 45.087 22.541 1.00 90.93 310 ND2 ASN C 42 17.611 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.611 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.474 48.926 49.006 1.00 10.51 327 N SER C 44 11.482 50.466 22.29.918 1.00 75.99 322 O ASN C 42 17.474 48.926 24.246 1.00 90.93 320 ND2 ASN C 42 17.651 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.651 45.087 22.641 1.00 90.93 321 C SER C 44 14.492 50.466 22.997 1.00 101.51 325 C G GLY C 43 16.315 48.394 22.096 1.00 101.51 326 C G GLY C 43 16.315 48.394 22.096 1.00 101.51 327 N SER C 44 14.492 50.466 22.907 1.00 101.51 328 C A SER C 44 13.183 50.282 2.007 1.00 101.51 329 CB SER C 44 13.183 50.282 2.007 1.00 101.51 326 C G GLY C 43 16.467 50.00 2.668 24.182 1.00 101.51 327 N SER C 44 14.492 50.466 22.907 1.00 101.51 326 C G GLY C 43 16.467 50.00 2.668 22.907 1.00 101.51 327 N SER C 44 11.866 48.962 25.114 1.00 19.93 330 OG SER C 44 13.183 50.282 2.007 1.00 101.51 326 C G GLY C 43 16.467 50.00 2.668 24.182 1.00 101.51 327 N SER C 44 11.866 48.962 25.114 1.00 11.51 328 CA SER C 44 11.866 48.962 25.114 1.00 11.51 327 N SER C 44 11.866 48.962 25.114 1.00 11.51 328 CA SER C 44 11.866 48.962 25.114 1.	25	299								
3002 CZ PHE C 40 11.003 51.853 30.130 1.00 132.74 303 CZ PHE C 40 11.002 51.501 31.344 1.00 132.74 303 CZ PHE C 40 13.225 46.677 27.474 1.00 81.86 305 N HIS C 41 12.761 46.239 26.314 1.00 70.61 306 CA HIS C 41 13.552 45.334 25.490 1.00 70.61 307 CB HIS C 41 13.552 45.334 25.490 1.00 70.61 308 CG HIS C 41 13.339 43.759 23.528 1.00 75.99 309 CD2 HIS C 41 13.192 43.567 22.188 1.00 75.99 310 ND1 HIS C 41 14.027 42.893 23.933 1.00 75.99 311 CEI HIS C 41 14.027 42.893 23.933 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.093 42.598 21.826 1.00 75.99 314 O HIS C 41 14.093 42.598 21.826 1.00 75.99 315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 316 CA ASN C 42 17.063 46.600 24.615 1.00 90.93 317 CB ASN C 42 17.063 46.600 24.615 1.00 90.93 318 CG ASN C 42 17.063 46.600 24.615 1.00 90.93 319 CD1 ASN C 42 17.063 46.403 23.085 1.00 90.93 320 ND2 ASN C 42 17.063 46.600 24.615 1.00 90.93 321 C ASN C 42 17.049 44.097 23.186 1.00 90.93 321 C ASN C 42 17.049 44.097 23.186 1.00 90.93 322 O ASN C 42 17.474 48.926 24.246 1.00 90.93 323 N GLY C 43 16.375 48.95 48.906 1.00 90.93 324 CA GLY C 43 16.375 48.95 48.906 1.00 101.51 325 C GLY C 43 16.276 50.666 38.077 24.971 1.00 90.99 322 O ASN C 42 17.474 48.926 24.246 1.00 90.93 323 N GLY C 43 16.375 48.95 48.906 1.00 101.51 326 O GLY C 43 16.375 50.672 22.641 1.00 101.51 327 N SER C 44 14.492 50.140 24.759 1.00 11.51 328 CA SER C 44 13.276 50.666 24.192 1.00 159.89 330 OG SER C 44 13.276 50.666 24.192 1.00 159.89 331 C SER C 44 13.276 50.666 24.192 1.00 159.89 332 OG SER C 44 13.276 50.666 24.31 1.00 11.51 327 N SER C 44 13.495 50.672 22.007 1.00 159.29 333 N LEU C 45 9.989 50.682 22.705 1.00 113.27 336 CB LEU C 45 9.989 50.682 22.705 1.00 113.27 336 CB LEU C 45 9.126 49.705 25.261 1.00 113.27 336 CB LEU C 45 9.126 49.705 25.261 1.00 113.27 336 CB LEU C 45 9.126 49.705 25.261 1.00 113.27 337 CD1 LEU C 45 9.126 49.705 25.261 1.00 113.27 340 O LEU C 45 9.126 49.705 25.261 1.00 113.27 341 N SER C 46 8.458 48.858 48.950 25.915 1.00 113.27					40	11.141	50.201			
303 C PHE C 40 11.020 51.501 31.344 1.00 132.74 30 304 O PHE C 40 13.225 46.677 27.474 1.00 81.86 305 N HIS C 41 12.761 46.239 26.314 1.00 70.61 307 CB HIS C 41 13.552 45.334 25.480 1.00 70.61 307 CB HIS C 41 13.3552 45.334 25.480 1.00 75.99 308 CG HIS C 41 13.399 43.759 23.528 1.00 75.99 310 ND1 HIS C 41 13.392 43.567 22.198 1.00 75.99 311 CEI HIS C 41 14.093 42.588 21.826 1.00 75.99 312 NE2 HIS C 41 14.093 42.588 21.826 1.00 75.99 313 C HIS C 41 14.671 46.118 24.794 1.00 75.99 311 CEI HIS C 41 14.671 46.118 24.794 1.00 75.99 312 NE2 HIS C 41 14.671 46.118 24.794 1.00 70.61 315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 316 CA ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.063 46.600 24.615 1.00 90.93 318 CG ASN C 42 17.194 44.097 23.186 1.00 90.93 320 ND2 ASN C 42 17.474 48.926 24.246 1.00 90.93 321 C ASN C 42 17.474 48.926 24.246 1.00 90.93 322 O ASN C 42 17.474 48.926 24.246 1.00 90.93 321 C SER C 44 13.495 51.235 26.721 1.00 90.99 322 O ASN C 42 17.474 48.926 24.246 1.00 90.93 321 C SER C 44 13.495 51.235 26.721 1.00 90.99 322 O ASN C 42 17.474 48.926 24.246 1.00 90.93 323 N GLY C 43 16.177 49.792 26.478 1.00 101.51 326 O G SER C 44 13.276 50.686 24.182 1.00 159.89 333 N LEU C 45 9.989 50.682 22.007 1.00 159.89 333 N LEU C 45 9.989 50.682 22.007 1.00 159.89 333 N LEU C 45 9.989 50.682 22.007 1.00 159.89 333 C SER C 44 13.276 50.686 24.821 1.00 101.51 326 C SER C 44 13.276 50.686 24.821 1.00 101.51 327 N SER C 44 13.276 50.686 24.821 1.00 159.89 333 N LEU C 45 9.989 50.682 28.091 1.00 113.27 336 CB LEU C 45 9.989 50.682 28.091 1.00 113.27 337 CD1 LEU C 45 9.989 50.682 28.091 1.00 113.27 338 CD2 LEU C 45 9.126 49.705 25.261 1.00 113.27 338 CD2 LEU C 45 9.126 49.705 25.261 1.00 113.27 339 CD3 SER C 44 13.276 50.686 47.83 25.007 1.00 113.27 331 N SER C 44 13.883 50.282 20.07 1.00 113.27 332 C SER C 44 12.046 50.168 24.931 1.00 113.27 333 C SER C 44 12.046 50.168 24.931 1.00 113.27 334 C SER C 46 8.488 48.88 48.88 25.915 1.00 113.27 335 CB LEU C 45 9.984 49.805 24.039 1.00 113.27 344 C C SER C 46 8								30.130		
300 304 O PHE C 40 14.321 46.333 27.917 1.00 81.86 305 N HIS C 41 12.761 46.239 26.314 1.00 70.61 306 CA HIS C 41 13.552 45.334 25.490 1.00 70.61 307 CB HIS C 41 12.633 44.671 24.470 1.00 75.99 308 CG HIS C 41 13.392 43.567 22.198 1.00 75.99 310 ND1 HIS C 41 13.192 43.567 22.198 1.00 75.99 311 CEI HIS C 41 14.327 42.883 23.933 1.00 75.99 311 CEI HIS C 41 14.765 42.207 22.892 1.00 75.99 312 NE2 HIS C 41 14.693 42.598 21.826 1.00 75.99 313 C HIS C 41 14.693 42.598 21.826 1.00 75.99 315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 316 C A ASN C 42 17.083 46.600 24.615 1.00 90.99 316 C A ASN C 42 17.108 46.600 24.615 1.00 90.99 318 CG ASN C 42 17.108 46.600 24.615 1.00 90.99 320 ND2 ASN C 42 17.161 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.160 48.463 23.085 1.00 90.93 320 ND2 ASN C 42 17.611 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.611 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.611 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.614 48.95 45.007 21.649 1.00 90.93 321 C ASN C 42 16.966 48.077 21.649 1.00 90.93 320 ND2 ASN C 42 17.614 48.95 45.007 21.649 1.00 90.93 321 C ASN C 42 16.966 48.077 24.971 1.00 90.99 322 N GLY C 43 16.315 48.394 26.086 1.00 101.51 325 C G GLY C 43 14.462 50.140 24.769 1.00 101.51 325 C G GLY C 43 14.265 51.235 26.721 1.00 101.51 325 C G GLY C 43 14.265 51.235 26.721 1.00 101.51 325 C G GLY C 43 14.265 51.235 26.721 1.00 101.51 325 C G GLY C 43 14.265 51.235 26.721 1.00 101.51 325 C G GLY C 43 14.265 51.235 26.721 1.00 101.51 326 C G GLY C 43 14.327 50.686 24.182 1.00 159.89 333 C G G GLU C 45 9.143 51.925 26.443 1.00 159.89 333 C G G GLU C 45 9.143 51.925 26.443 1.00 113.27 336 C G G GLU C 45 9.989 50.882 26.091 1.00 113.27 336 C G G GLU C 45 9.143 51.925 26.443 1.00 113.27 336 C G G GLU C 45 9.989 50.882 26.091 1.00 113.27 336 C G G GLU C 45 9.143 51.925 26.443 1.00 113.27 336 C G G GLU C 45 9.143 51.925 26.443 1.00 113.27 336 C G G GLU C 45 9.989 50.882 26.091 1.00 113.27 336 C G G GLU C 45 9.989 50.882 25.014 1.00 113.27 336 C G G GLU C 45 9.989 50.882 25.014 1.00 113.27 336 C G G G										
305 N HIS C 41 12.761 46.239 25.314 1.00 70.61 306 CA HIS C 41 13.552 45.334 25.490 1.00 70.61 307 CB HIS C 41 13.552 45.334 4.671 24.470 1.00 75.99 308 CG HIS C 41 13.339 43.759 23.528 1.00 75.99 310 ND1 HIS C 41 13.339 43.759 23.528 1.00 75.99 310 ND1 HIS C 41 14.27 42.883 23.933 1.00 75.99 311 CEI HIS C 41 14.765 42.207 22.892 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 312 NE2 HIS C 41 14.671 46.118 24.794 1.00 70.61 315 N ASN C 41 14.408 46.922 23.918 1.00 70.61 315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 317 CB ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.150 46.463 23.085 1.00 90.99 317 CB ASN C 42 17.150 46.463 23.085 1.00 90.99 317 CB ASN C 42 17.149 44.097 23.168 1.00 90.93 320 ND2 ASN C 42 17.491 44.097 23.168 1.00 90.93 321 C ASN C 42 17.419 44.097 23.168 1.00 90.93 321 C ASN C 42 18.495 45.007 21.649 1.00 90.93 321 C ASN C 42 17.474 48.926 24.246 1.00 90.93 321 C ASN C 42 17.474 48.926 24.246 1.00 90.93 322 C ASN C 42 17.474 48.926 24.246 1.00 90.93 323 N GLY C 43 16.315 48.394 28.086 1.00 101.51 327 N SER C 44 13.276 50.686 24.182 1.00 101.51 327 N SER C 44 13.276 50.686 24.182 1.00 101.51 327 N SER C 44 13.276 50.686 24.182 1.00 159.89 333 N LEU C 45 9.969 50.882 22.2705 1.00 101.51 327 N SER C 44 13.83 50.282 22.705 1.00 101.51 327 N SER C 44 13.83 50.282 22.705 1.00 101.51 327 N SER C 44 13.86 48.962 24.182 1.00 159.89 332 C SER C 44 13.86 48.962 25.114 1.00 159.89 333 N LEU C 45 9.969 50.882 26.091 1.00 159.89 333 N LEU C 45 9.969 50.882 26.091 1.00 159.89 333 C C LEU C 45 9.969 50.882 26.091 1.00 113.27 337 CD1 LEU C 45 9.969 50.882 26.091 1.00 113.27 337 CD1 LEU C 45 9.969 50.882 26.091 1.00 113.27 337 CD1 LEU C 45 9.969 50.882 26.091 1.00 113.27 337 CD1 LEU C 45 9.969 50.882 26.091 1.00 113.27 338 CC2 LEU C 45 9.148 49.905 24.039 1.00 127.30 340 O LEU C 45 9.084 49.805 24.039 1.00 127.30 342 CA SER C 46 7.636 47.802 49.400 25.829 1.00 104.59 342 CA SER C 46 7.6	30								1.00	
306 CA HIS C 41 13.552 45.334 25.490 1.00 70.61 307 CB HIS C 41 12.633 44.671 24.470 1.00 75.99 308 CG HIS C 41 13.339 43.759 23.528 1.00 75.99 310 ND1 HIS C 41 14.327 42.883 23.933 1.00 75.99 311 CEI HIS C 41 14.327 42.883 23.933 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.093 42.598 21.826 1.00 75.99 315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 316 CA ASN C 42 17.150 46.463 23.095 1.00 90.93 317 CB ASN C 42 17.150 46.463 23.095 1.00 90.93 318 CG ASN C 42 17.150 46.463 23.095 1.00 90.93 320 ND2 ASN C 42 17.150 46.463 23.095 1.00 90.93 321 C ASN C 42 17.474 48.926 24.261 1.00 90.93 321 C ASN C 42 17.474 48.926 24.261 1.00 90.93 321 C ASN C 42 17.474 48.926 24.261 1.00 90.93 321 C ASN C 42 17.474 48.926 24.246 1.00 90.93 321 C ASN C 42 17.474 48.926 24.246 1.00 90.93 321 C ASN C 42 17.474 48.926 24.246 1.00 90.93 321 C ASN C 42 17.474 48.926 24.246 1.00 90.93 322 C ASN C 42 17.474 48.926 24.246 1.00 90.93 322 C ASN C 42 17.474 48.926 24.246 1.00 90.93 322 C ASN C 42 17.474 48.926 24.246 1.00 90.93 322 C ASN C 42 17.475 48.936 24.246 1.00 90.93 322 C ASN C 42 17.475 48.936 24.246 1.00 90.93 322 C ASN C 42 17.475 48.936 24.246 1.00 90.93 322 C ASN C 42 17.475 48.926 24.246 1.00 90.93 322 C ASN C 42 17.475 48.926 24.246 1.00 90.93 322 C ASN C 42 17.475 48.926 24.246 1.00 90.93 322 C ASR C 44 14.492 50.140 24.769 1.00 101.51 325 C C GLY C 43 14.09 50.466 25.997 1.00 101.51 326 C C GLY C 43 14.09 50.466 25.997 1.00 101.51 327 N SER C 44 13.276 50.686 24.182 1.00 101.51 327 329 CB SER C 44 13.276 50.686 24.182 1.00 101.51 327 329 CB SER C 44 13.276 50.686 24.182 1.00 101.51 327 333 C C EC 44 13.886 48.982 25.114 1.00 159.89 333 N LEU C 45 9.999 50.682 26.091 1.00 153.29 334 CA LEU C 45 9.999 50.682 26.091 1.00 153.29 336 C LEU C 45 9.999 50.682 26.091 1.00 172.30 340 O LEU C 45 9.909 50.682 26.091 1.00 172.30 340 O LEU C 45 9.929 50.682 26.091 1.00 172.30 341 N SER C 46 8.858 48.758 25.915	50									
307 CB HIS C 41 12.633 44.671 24.470 1.00 75.99 308 CG HIS C 41 13.339 43.759 23.528 1.00 75.99 310 ND1 HIS C 41 13.3192 43.567 22.188 1.00 75.99 311 CE1 HIS C 41 14.327 42.893 23.933 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 313 CE1 HIS C 41 14.093 42.598 21.826 1.00 75.99 314 O HIS C 41 14.671 46.118 24.794 1.00 70.61 315 N ASN C 41 14.08 46.922 23.918 1.00 70.61 316 CA ASN C 42 15.916 45.879 25.177 1.00 90.99 317 CB ASN C 42 17.063 46.600 24.615 1.00 90.93 318 CG ASN C 42 17.651 45.087 22.641 1.00 90.93 319 OD1 ASN C 42 17.611 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.611 45.087 22.641 1.00 90.93 321 C ASN C 42 17.419 44.097 21.3186 1.00 90.93 322 O ASN C 42 16.966 48.077 21.649 1.00 90.93 323 N GLY C 43 16.315 48.394 26.086 1.00 90.93 323 N GLY C 43 16.315 48.394 26.086 1.00 101.51 326 O GLY C 43 16.315 48.394 26.086 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 101.51 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 330 CG LEU C 45 9.969 50.882 22.007 1.00 159.89 331 C SER C 44 11.3276 50.686 24.931 1.00 159.89 332 CA LEU C 45 9.969 50.882 22.705 1.00 159.89 333 N LEU C 45 9.969 50.882 22.007 1.00 159.89 334 CA LEU C 45 9.969 50.882 22.007 1.00 159.89 335 CB LEU C 45 9.969 50.882 26.091 1.00 11.327 337 CD1 LEU C 45 9.969 50.882 26.091 1.00 11.327 338 CD2 LEU C 45 9.969 50.882 26.091 1.00 113.27 337 CD1 LEU C 45 9.969 50.882 26.091 1.00 113.27 338 CD2 LEU C 45 9.969 50.882 26.091 1.00 113.27 337 CD1 LEU C 45 9.969 50.882 26.091 1.00 113.27 338 CD2 LEU C 45 9.969 50.882 26.091 1.00 113.27 339 CD2 LEU C 45 9.969 50.882 26.091 1.00 113.27 339 CD3 LEU C 45 9.969 50.882 26.091 1.00 127.30 340 O LEU C 45 9.084 49.805 24.039 1.00 113.27 341 N SER C 46 8.458 48.758 25.915 1.00 104.59										
308										
309 CD2 HIS C 41 13.192 43.567 22.198 1.00 75.99 310 ND1 HIS C 41 14.327 42.883 23.933 1.00 75.99 311 CE1 HIS C 41 14.765 42.207 22.892 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.093 42.598 21.826 1.00 75.99 314 O HIS C 41 14.093 42.598 21.826 1.00 75.99 315 N ASN C 42 11.409 46.118 24.794 1.00 70.61 316 CA ASN C 42 15.916 45.879 25.177 1.00 90.99 317 CB ASN C 42 17.063 46.600 24.615 1.00 90.93 318 CG ASN C 42 17.063 46.600 24.615 1.00 90.93 319 OD1 ASN C 42 17.150 46.463 22.085 1.00 90.93 320 ND2 ASN C 42 17.151 45.087 22.641 1.00 90.93 321 C ASN C 42 18.495 45.007 21.649 1.00 90.93 322 O ASN C 42 16.966 48.077 24.971 1.00 90.99 323 N GLY C 43 16.315 48.394 26.086 1.00 90.99 324 CA GLY C 43 16.315 48.394 26.086 1.00 101.51 325 C GLY C 43 14.2.9 50.456 25.997 1.00 101.51 326 O GLY C 43 14.2.9 50.456 25.997 1.00 101.51 327 N SER C 44 14.492 50.440 24.769 1.00 159.89 329 CB SER C 44 13.183 50.282 22.705 1.00 159.89 320 ND LEU C 45 9.989 50.682 25.114 1.00 159.89 321 C SER C 44 13.183 50.282 22.705 1.00 159.89 322 O SER C 44 13.183 50.282 22.705 1.00 159.89 323 C BER C 44 13.183 50.282 22.705 1.00 159.89 324 CA LEU C 45 9.989 50.682 25.114 1.00 159.89 325 CB LEU C 45 9.989 50.682 25.114 1.00 159.89 326 CB SER C 44 11.886 48.982 25.114 1.00 159.89 327 N SER C 44 11.886 48.982 25.114 1.00 159.89 328 CA SER C 44 13.183 50.282 22.705 1.00 159.89 329 CB SER C 44 11.886 48.982 25.114 1.00 159.89 329 CB SER C 44 11.886 48.982 25.114 1.00 159.89 320 ND LEU C 45 9.143 51.925 26.443 1.00 113.27 337 CD1 LEU C 45 9.143 51.925 26.403 1.00 113.27 338 CD2 LEU C 45 9.143 51.925 26.403 1.00 113.27 339 CD2 LEU C 45 9.126 49.705 25.261 1.00 113.27 339 CD2 LEU C 45 9.126 49.705 25.261 1.00 113.27 339 CD2 LEU C 45 9.084 49.805 24.039 1.00 113.27 340 O LEU C 45 9.084 49.805 24.039 1.00 127.30 341 N SER C 46 7.802 46.400 25.829 1.00 104.59				HIS C						
310 ND1 HIS C 41 14.327 42.883 23.933 1.00 75.99 311 CE1 HIS C 41 14.765 42.207 22.882 1.00 75.99 312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.093 42.598 21.826 1.00 70.61 315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 316 CA ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.063 46.600 24.615 1.00 90.99 318 CG ASN C 42 17.150 46.483 23.085 1.00 90.93 319 OD1 ASN C 42 17.150 46.483 23.085 1.00 90.93 320 ND2 ASN C 42 17.149 44.097 23.186 1.00 90.93 321 C ASN C 42 17.149 44.097 23.186 1.00 90.93 322 O ASN C 42 17.474 48.926 24.246 1.00 90.99 323 N GLY C 43 16.315 48.394 26.086 1.00 101.51 326 O GLY C 43 16.315 48.394 26.086 1.00 101.51 327 N SER C 44 14.492 50.440 24.769 1.00 101.51 327 N SER C 44 14.492 50.440 24.769 1.00 101.51 327 N SER C 44 13.183 50.282 22.705 1.00 159.89 330 OG SER C 44 13.276 50.686 24.182 1.00 159.89 331 C SER C 44 13.875 50.612 22.007 1.00 159.89 332 C LEU C 45 9.143 51.025 22.561 1.00 159.89 333 N LEU C 45 9.143 51.025 22.561 1.00 159.89 334 CA LEU C 45 9.143 51.025 22.561 1.00 159.89 335 CB LEU C 45 9.143 51.025 22.561 1.00 159.89 337 CD1 LEU C 45 9.143 51.025 22.561 1.00 13.27 338 CD2 LEU C 45 9.143 51.025 22.561 1.00 13.27 339 C LEU C 45 9.143 51.025 22.561 1.00 13.27 337 CD1 LEU C 45 9.143 51.025 22.561 1.00 13.27 338 CD2 LEU C 45 9.143 51.025 22.561 1.00 13.27 339 C LEU C 45 9.143 51.025 22.561 1.00 13.27 337 CD1 LEU C 45 9.143 51.025 22.561 1.00 13.27 338 CD2 LEU C 45 9.143 51.025 22.561 1.00 13.27 339 C LEU C 45 9.143 51.025 22.561 1.00 13.27 339 C C LEU C 45 9.143 51.025 22.561 1.00 13.27 337 CD1 LEU C 45 9.126 49.705 25.266 1.00 13.27 339 C C LEU C 45 9.143 51.025 22.561 1.00 13.27 337 CD1 LEU C 45 9.126 49.805 25.501 1.00 13.27 338 CD2 LEU C 45 9.143 51.025 22.561 1.00 13.27 339 C C LEU C 45 9.143 51.025 22.561 1.00 13.27 330 CD SER C 46 7.802 47.802 47.803 1.00 13.27 337 CD1 LEU C 45 9.126 49.805 25.501 1.00 13.27 340 C LEU C 45 9.044 49.805 25.561 1.00 104.59	35	309	CD2							
311 CE1 HIS C 41 14.765 42.207 22.892 1.00 75.99 313 C HIS C 41 14.093 42.598 21.826 1.00 75.99 313 C HIS C 41 14.671 46.118 24.794 1.00 70.61 314 O HIS C 41 14.671 46.118 24.794 1.00 70.61 315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 316 CA ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.150 46.483 23.085 1.00 90.99 318 CG ASN C 42 17.150 46.483 23.085 1.00 90.93 318 CG ASN C 42 17.150 46.483 23.085 1.00 90.93 320 ND2 ASN C 42 17.149 44.097 23.166 1.00 90.93 321 C ASN C 42 17.411 45.087 22.641 1.00 90.93 322 O ASN C 42 18.495 45.007 21.649 1.00 90.93 323 N GLY C 43 16.315 48.394 26.086 1.00 90.99 323 N GLY C 43 16.315 48.394 26.086 1.00 101.51 325 C GLY C 43 14.265 51.235 26.721 1.00 101.51 326 O GLY C 43 14.265 51.235 26.721 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 101.51 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 329 CB SER C 44 13.276 50.686 24.182 1.00 159.89 330 OG SER C 44 13.183 50.282 22.705 1.00 159.89 331 C SER C 44 11.886 48.962 25.114 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 9.969 50.682 26.091 1.00 159.89 334 CA LEU C 45 9.969 50.682 26.091 1.00 159.89 335 CB LEU C 45 9.969 50.682 26.091 1.00 13.27 337 CD1 LEU C 45 9.143 51.925 26.443 1.00 13.27 338 CD2 LEU C 45 9.969 50.682 26.091 1.00 13.27 339 C LEU C 45 9.969 50.682 26.091 1.00 13.27 339 C LEU C 45 9.969 50.682 26.091 1.00 13.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 13.27 339 C C LEU C 45 9.969 50.682 26.091 1.00 13.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 13.27 339 C C LEU C 45 9.969 50.682 26.091 1.00 13.27 339 C C LEU C 45 9.126 49.705 25.261 1.00 13.27 339 C C LEU C 45 7.210 53.024 27.553 1.00 13.27 339 C C LEU C 45 7.210 53.024 27.553 1.00 13.27 331 N SER C 46 8.858 48.758 25.915 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 145.59					41					
312 NE2 HIS C 41 14.093 42.598 21.826 1.00 75.99 40 314 O HIS C 41 14.671 46.118 24.794 1.00 70.61 315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 316 CA ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.150 46.463 23.085 1.00 90.93 318 CG ASN C 42 17.150 46.463 23.085 1.00 90.93 319 OD1 ASN C 42 17.149 44.097 23.186 1.00 90.93 320 ND2 ASN C 42 17.149 44.097 23.186 1.00 90.93 321 C ASN C 42 16.966 48.077 24.971 1.00 90.93 322 O ASN C 42 17.474 48.926 24.246 1.00 90.99 323 N GLY C 43 16.315 48.394 28.086 1.00 101.51 325 C GLY C 43 16.177 49.792 26.478 1.00 101.51 326 O GLY C 43 16.177 49.792 26.478 1.00 101.51 327 N SER C 44 14.295 50.466 25.997 1.00 101.51 328 CA SER C 44 13.276 50.686 24.182 1.00 105.989 330 OG SER C 44 13.276 50.686 24.182 1.00 159.89 331 C SER C 44 13.276 50.686 24.182 1.00 159.89 332 O SER C 44 12.046 50.168 24.931 1.00 159.89 333 N LEU C 45 9.969 50.682 25.114 1.00 159.89 333 N LEU C 45 9.969 50.682 25.114 1.00 159.89 333 N LEU C 45 9.969 50.682 26.091 1.00 159.89 333 CG LEU C 45 9.969 50.682 26.091 1.00 127.30 340 O LEU C 45 9.969 50.682 26.091 1.00 13.27 336 CG LEU C 45 9.969 50.682 26.091 1.00 13.27 337 CD1 LEU C 45 9.969 50.682 26.091 1.00 13.27 338 CD2 LEU C 45 9.184 49.805 24.039 1.00 13.27 339 C BER C 44 13.83 51.925 25.6443 1.00 13.27 331 N SER C 45 9.143 51.925 25.261 1.00 13.27 332 CB LEU C 45 9.969 50.682 26.091 1.00 13.27 334 CA SER C 45 9.143 51.925 25.6443 1.00 13.27 335 CB LEU C 45 9.969 50.682 26.091 1.00 13.27 336 CG LEU C 45 9.184 49.805 24.039 1.00 13.27 337 CD1 LEU C 45 9.184 49.805 24.039 1.00 127.30 340 O LEU C 45 9.126 49.705 25.261 1.00 127.30 341 N SER C 46 8.485 48.758 25.915 1.00 104.59 343 CB SER C 46 7.836 48.758 25.915 1.00 104.59 344 CA SER C 46 7.836 48.758 25.950 1.00 104.59						14.765	42.207			
40 314 O HIS C 41 14.408 46.922 23.918 1.00 70.61 315 N ASN C 42 15.916 45.879 25.177 1.00 80.89 317 CB ASN C 42 17.163 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.150 46.463 23.085 1.00 90.93 318 CG ASN C 42 17.150 46.463 23.085 1.00 90.93 318 CG ASN C 42 17.161 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.149 44.097 23.186 1.00 90.93 321 C ASN C 42 17.149 44.097 23.186 1.00 90.93 321 C ASN C 42 16.966 48.077 24.971 1.00 90.99 322 O ASN C 42 16.966 48.077 24.971 1.00 90.99 322 O ASN C 42 16.966 48.077 24.971 1.00 90.99 322 C ASN C 42 16.966 48.077 24.971 1.00 90.99 323 N GLY C 43 16.315 48.394 28.086 1.00 101.51 325 C GLY C 43 14.2.9 50.456 51.235 26.086 1.00 101.51 325 C GLY C 43 14.2.9 50.456 51.235 26.721 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 101.51 327 N SER C 44 13.183 50.282 22.705 1.00 159.89 330 CG SER C 44 13.183 50.282 22.705 1.00 153.29 331 C SER C 44 13.183 50.282 22.705 1.00 153.29 332 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 C SER C 44 12.046 50.168 24.931 1.00 159.89 333 N LEU C 45 9.969 50.682 24.931 1.00 159.89 332 CG LEU C 45 9.969 50.682 26.091 1.00 13.27 30 335 CB LEU C 45 9.969 50.682 26.091 1.00 13.27 336 CG LEU C 45 9.969 50.682 26.091 1.00 13.27 337 CD1 LEU C 45 9.143 51.925 26.443 1.00 13.27 337 CD1 LEU C 45 9.969 50.682 26.091 1.00 13.27 337 CD1 LEU C 45 9.163 49.805 24.039 1.00 13.27 337 CD1 LEU C 45 9.163 49.805 24.039 1.00 13.27 337 CD1 LEU C 45 9.164 49.805 24.039 1.00 13.27 337 CD1 LEU C 45 9.164 49.805 24.039 1.00 13.27 337 CD1 LEU C 45 9.164 49.805 24.039 1.00 13.27 3340 C LEU C 45 9.164 49.805 24.039 1.00 13.27 3341 N SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.63								21.826	1.00	
315 N ASN C 42 15.916 45.879 25.177 1.00 90.99 316 CA ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.150 46.463 23.085 1.00 90.99 318 CG ASN C 42 17.150 46.463 23.085 1.00 90.93 318 CG ASN C 42 17.149 44.097 23.186 1.00 90.93 320 ND2 ASN C 42 17.149 44.097 23.186 1.00 90.93 321 C ASN C 42 18.495 45.007 21.649 1.00 90.93 322 O ASN C 42 18.495 45.007 21.649 1.00 90.93 323 N GLY C 43 16.315 48.394 26.086 1.00 90.99 324 CA GLY C 43 16.315 48.394 26.086 1.00 101.51 325 C GLY C 43 14.6.79 50.456 25.997 1.00 101.51 326 O GLY C 43 14.6.95 50.456 25.997 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 105.989 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 330 OG SER C 44 13.276 50.686 24.182 1.00 159.89 331 C SER C 44 13.276 50.686 24.182 1.00 159.89 332 O SER C 44 12.046 50.168 24.931 1.00 159.89 333 N LEU C 45 9.969 50.682 25.114 1.00 159.89 333 C SER C 44 12.046 50.168 24.931 1.00 159.89 333 C SER C 44 12.046 50.168 24.931 1.00 159.89 333 C SER C 44 12.046 50.168 24.931 1.00 159.89 333 C SER C 44 12.046 50.168 24.931 1.00 159.89 333 C SER C 44 12.046 50.168 24.931 1.00 159.89 333 C SER C 44 12.046 50.168 24.931 1.00 159.89 333 C SER C 44 12.046 50.168 24.931 1.00 159.89 334 CA LEU C 45 9.969 50.682 25.114 1.00 159.89 335 CB LEU C 45 9.969 50.682 25.114 1.00 159.89 336 CG LEU C 45 9.969 50.682 25.114 1.00 159.89 337 CD1 LEU C 45 9.969 50.682 25.114 1.00 13.27 338 CD2 LEU C 45 9.166 49.705 25.268 1.00 113.27 337 CD1 LEU C 45 9.166 49.705 25.261 1.00 113.27 338 CD2 LEU C 45 9.166 49.705 25.261 1.00 113.27 337 CD1 LEU C 45 9.166 49.705 25.261 1.00 113.27 338 CD2 LEU C 45 9.126 49.705 25.261 1.00 127.30 341 N SER C 46 7.836 47.784 25.206 1.00 104.59 343 CB SER C 46 7.836 47.784 25.206 1.00 104.59	40									
316 CA ASN C 42 17.063 46.600 24.615 1.00 90.99 317 CB ASN C 42 17.150 46.463 23.085 1.00 90.93 318 CG ASN C 42 17.611 45.087 22.641 1.00 90.93 320 ND2 ASN C 42 17.149 44.097 23.186 1.00 90.93 321 C ASN C 42 18.495 45.007 21.649 1.00 90.93 322 O ASN C 42 16.966 48.077 24.971 1.00 90.93 323 N GLY C 43 16.315 48.394 26.086 1.00 101.51 324 CA GLY C 43 16.177 49.792 26.478 1.00 101.51 325 C GLY C 43 14.6.9 50.466 25.997 1.00 101.51 326 O GLY C 43 14.265 51.235 26.721 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 105.989 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 329 CB SER C 44 13.276 50.686 24.182 1.00 159.89 330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 333 N LEU C 45 9.969 50.682 26.091 1.00 127.30 336 CG LEU C 45 7.855 51.691 27.238 1.00 113.27 337 CD1 LEU C 45 9.969 50.682 26.091 1.00 127.30 340 O LEU C 45 9.126 49.705 25.261 1.00 132.27 337 CD1 LEU C 45 9.126 49.705 25.261 1.00 132.27 338 CD2 LEU C 45 9.126 49.705 25.261 1.00 132.27 339 C LEU C 45 9.126 49.705 25.261 1.00 132.27 339 C LEU C 45 9.126 49.705 25.261 1.00 132.27 339 C LEU C 45 9.126 49.705 25.261 1.00 132.27 339 C LEU C 45 9.126 49.705 25.261 1.00 132.27 340 O LEU C 45 9.126 49.705 25.261 1.00 132.27 341 N SER C 46 7.636 47.784 25.206 1.00 132.27 341 N SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 344 CA SER C 46 7.636 47.784 25.206 1.00 104.59 344 CA SER C 46 7.636 47.784 25.206 1.00 104.59 344 CA SER C 46 7.636 47.784 25.206 1.00 104.59	TU									
317 CB ASN C 42 17.150 46.463 23.085 1.00 90.93 318 CG ASN C 42 17.611 45.087 22.641 1.00 90.93 319 OD1 ASN C 42 17.149 44.097 23.166 1.00 90.93 320 ND2 ASN C 42 18.495 45.007 21.649 1.00 90.93 321 C ASN C 42 16.966 48.077 24.971 1.00 90.99 322 O ASN C 42 16.966 48.077 24.971 1.00 90.99 323 N GLY C 43 16.315 48.394 28.086 1.00 101.51 325 C GLY C 43 16.177 49.792 26.478 1.00 101.51 326 O GLY C 43 14.6.9 50.466 25.997 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 101.51 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 329 CB SER C 44 13.183 50.282 22.705 1.00 159.89 330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 9.969 50.682 25.114 1.00 159.89 334 CA LEU C 45 9.969 50.682 25.114 1.00 159.89 335 CB LEU C 45 9.969 50.682 26.091 1.00 127.30 336 CG LEU C 45 9.143 51.925 26.443 1.00 132.27 337 CD1 LEU C 45 9.143 51.925 26.443 1.00 132.27 338 CD2 LEU C 45 9.143 51.925 26.443 1.00 132.27 339 C LEU C 45 9.143 51.925 26.443 1.00 132.27 339 C LEU C 45 9.143 51.925 26.443 1.00 132.27 330 CD LEU C 45 9.143 51.925 26.443 1.00 132.27 337 CD1 LEU C 45 9.143 51.925 26.443 1.00 132.27 338 CD2 LEU C 45 9.143 51.925 26.443 1.00 132.27 339 CD LEU C 45 9.143 51.925 26.443 1.00 132.27 330 CD LEU C 45 9.143 51.925 26.443 1.00 132.27 330 CD LEU C 45 9.143 51.925 26.443 1.00 132.27 331 N LEU C 45 9.969 50.682 26.091 1.00 132.27 332 CD LEU C 45 9.143 51.925 26.443 1.00 132.27 338 CD2 LEU C 45 9.143 51.925 26.443 1.00 132.27 339 CD LEU C 45 9.144 49.805 24.039 1.00 132.27 340 CD LEU C 45 9.084 49.805 24.039 1.00 127.30 341 N SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59										
45 318										
45 319 OD1 ASN C 42 17.149 44.097 23.186 1.00 90.93 320 ND2 ASN C 42 18.495 45.007 21.649 1.00 90.93 321 C ASN C 42 16.966 48.077 24.971 1.00 90.99 322 O ASN C 42 17.474 48.926 24.246 1.00 90.99 323 N GLY C 43 16.315 48.394 26.086 1.00 101.51 324 CA GLY C 43 16.177 49.782 26.478 1.00 101.51 325 C GLY C 43 14.0.9 50.456 25.997 1.00 101.51 326 O GLY C 43 14.265 51.235 26.721 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 159.89 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 329 CB SER C 44 13.183 50.282 22.705 1.00 159.89 330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 9.969 50.682 26.091 1.00 159.89 334 CA LEU C 45 9.969 50.682 26.091 1.00 127.30 335 CB LEU C 45 9.969 50.682 26.091 1.00 127.30 336 CG LEU C 45 9.143 51.925 26.443 1.00 113.27 337 CD1 LEU C 45 9.969 50.682 26.091 1.00 127.30 338 CD2 LEU C 45 7.855 51.691 27.238 1.00 113.27 339 CD LEU C 45 9.167 50.902 28.502 1.00 113.27 339 CD LEU C 45 9.167 50.002 28.502 1.00 113.27 339 CD LEU C 45 9.166 49.705 25.261 1.00 127.30 340 O LEU C 45 9.126 49.705 25.261 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 127.30 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 344 CA SER C 46 7.636 47.784 25.206 1.00 104.59										
320 ND2 ASN C 42 18.495 45.007 21.649 1.00 90.93 321 C ASN C 42 16.966 48.077 24.971 1.00 90.99 322 O ASN C 42 17.474 48.926 24.246 1.00 90.99 323 N GLY C 43 16.315 48.394 26.086 1.00 101.51 325 C GLY C 43 14.6.9 50.456 25.997 1.00 101.51 326 O GLY C 43 14.6.9 50.456 25.997 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 101.51 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 330 OG SER C 44 13.183 50.282 22.705 1.00 159.89 331 C SER C 44 14.375 50.612 22.007 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 11.179 51.076 25.368 1.00 127.30 335 CB LEU C 45 9.969 50.682 26.091 1.00 127.30 336 CG LEU C 45 9.143 51.925 26.443 1.00 113.27 337 CD1 LEU C 45 9.143 51.925 26.443 1.00 113.27 338 CD2 LEU C 45 9.143 51.925 26.443 1.00 113.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 113.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 113.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 113.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 113.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 113.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 113.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 113.27 339 C C LEU C 45 9.143 51.925 26.443 1.00 113.27 340 O LEU C 45 9.126 49.705 25.261 1.00 113.27 341 N SER C 46 7.636 49.705 25.261 1.00 127.30 341 N SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59	45	319	OD1							
321			ND2		42					
322							48.077			
50 324 CA GLY C 43 16.177 49.792 26.478 1.00 101.51 325 C GLY C 43 14.6.9 50.456 25.997 1.00 101.51 326 O GLY C 43 14.265 51.235 26.721 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 159.89 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 329 CB SER C 44 13.183 50.282 22.705 1.00 153.29 330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 11.179 51.076 25.368 1.00 127.30 335 CB LEU C 45 9.969 50.682 26.091 1.00 127.30 335 CB LEU C 45 9.969 50.682 26.091 1.00 127.30 335 CB LEU C 45 9.969 50.682 26.091 1.00 113.27 336 CG LEU C 45 9.143 51.925 26.443 1.00 113.27 337 CD1 LEU C 45 9.143 51.925 26.443 1.00 113.27 337 CD1 LEU C 45 9.143 51.925 26.443 1.00 113.27 338 CD2 LEU C 45 9.143 51.925 26.443 1.00 113.27 337 CD1 LEU C 45 9.126 49.705 25.261 1.00 113.27 340 O LEU C 45 9.126 49.705 25.261 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 127.30 342 CA SER C 46 7.636 47.784 25.206 1.00 127.30 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 120.90								24.246		
325	50									
326 O GLY C 43 14.265 51.235 26.721 1.00 101.51 327 N SER C 44 14.492 50.140 24.769 1.00 159.89 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 329 CB SER C 44 13.183 50.282 22.705 1.00 153.29 330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 11.179 51.076 25.368 1.00 127.30 335 CA LEU C 45 9.969 50.682 26.091 1.00 127.30 335 CB LEU C 45 9.143 51.925 26.443 1.00 113.27 336 CG LEU C 45 9.143 51.925 26.443 1.00 113.27 337 CD1 LEU C 45 8.167 50.902 28.502 1.00 113.27 338 CD2 LEU C 45 7.210 53.024 27.593 1.00 113.27 339 C LEU C 45 9.164 49.805 24.039 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.630 46.400 25.829 1.00 120.90	50									
327 N SER C 44 14.492 50.140 24.769 1.00 159.89 328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 329 CB SER C 44 13.183 50.282 22.705 1.00 153.29 330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 11.179 51.076 25.368 1.00 127.30 336 CA LEU C 45 9.969 50.682 26.091 1.00 127.30 337 CD1 LEU C 45 9.143 51.925 26.443 1.00 113.27 338 CG LEU C 45 7.855 51.691 27.238 1.00 113.27 339 C C LEU C 45 7.210 53.024 27.593 1.00 113.27 339 C C LEU C 45 9.126 49.705 25.261 1.00 113.27 340 O LEU C 45 9.126 49.705 25.261 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 127.30 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59 344 CB SER C 46 7.630 47.784 25.206 1.00 104.59										
328 CA SER C 44 13.276 50.686 24.182 1.00 159.89 329 CB SER C 44 13.183 50.282 22.705 1.00 153.29 330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 11.179 51.076 25.368 1.00 127.30 334 CA LEU C 45 9.969 50.682 26.091 1.00 127.30 335 CB LEU C 45 9.143 51.925 26.443 1.00 113.27 336 CG LEU C 45 8.167										
55 329 CB SER C 44 13.183 50.282 22.705 1.00 153.29 330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 11.179 51.076 25.368 1.00 127.30 335 CB LEU C 45 9.143 51.925 26.443 1.00 113.27 336 CG LEU C 45 7.855 51.691 27.238 1.00 113.27 337 CD1 LEU C 45 7.210 53.024 27.593 1.00 113.27 65 339 C LEU C 45 </td <td></td> <td>328</td> <td>CA</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>		328	CA							
330 OG SER C 44 14.375 50.612 22.007 1.00 153.29 331 C SER C 44 12.046 50.168 24.931 1.00 159.89 332 O SER C 44 11.886 48.962 25.114 1.00 159.89 333 N LEU C 45 11.179 51.076 25.368 1.00 127.30 335 CB LEU C 45 9.969 50.682 26.091 1.00 127.30 336 CG LEU C 45 9.143 51.925 26.443 1.00 113.27 336 CG LEU C 45 7.855 51.691 27.238 1.00 113.27 337 CD1 LEU C 45 8.167 50.902 28.502 1.00 113.27 338 CD2 LEU C 45 7.210 53.024 27.593 1.00 113.27 339 C LEU C 45 9.126 49.705 25.2661 1.00 127.30 340 O LEU C 45 9.126 49.705 25.261 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59	55		CB							
331					44					
60 334							50.168	24.931		
60 334 CA LEU C 45 9.969 50.682 26.091 1.00 127.30 335 CB LEU C 45 9.143 51.925 26.443 1.00 113.27 336 CG LEU C 45 7.855 51.691 27.238 1.00 113.27 337 CD1 LEU C 45 8.167 50.902 28.502 1.00 113.27 338 CD2 LEU C 45 7.210 53.024 27.593 1.00 113.27 339 C LEU C 45 9.126 49.705 25.261 1.00 127.30 340 O LEU C 45 9.126 49.805 25.261 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 120.90									1.00	
335 CB LEU C 45 9.143 51.925 26.443 1.00 113.27 336 CG LEU C 45 7.855 51.691 27.238 1.00 113.27 337 CD1 LEU C 45 8.167 50.902 28.502 1.00 113.27 338 CD2 LEU C 45 7.210 53.024 27.593 1.00 113.27 339 C LEU C 45 9.126 49.705 25.261 1.00 127.30 340 O LEU C 45 9.126 49.705 25.261 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.636 47.784 25.206 1.00 104.59	60									
336	•			LEU C						
337 CD1 LEU C 45 8.167 50.902 28.502 1.00 113.27 338 CD2 LEU C 45 7.210 53.024 27.593 1.00 113.27 65 339 C LEU C 45 9.126 49.705 25.261 1.00 127.30 340 O LEU C 45 9.084 49.805 24.039 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.802 46.400 25.829 1.00 120.90										
338 CD2 LEU C 45 7.210 53.024 27.593 1.00 113.27 339 C LEU C 45 9.126 49.705 25.261 1.00 127.30 340 O LEU C 45 9.084 49.805 24.039 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.802 46.400 25.829 1.00 120.90										
05 339 C LEU C 45 9.126 49.705 25.261 1.00 127.30 340 O LEU C 45 9.084 49.805 24.039 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.802 46.400 25.829 1.00 120.90		338	CD2	LEU C						
340 O LEU C 45 9.084 49.805 24.039 1.00 127.30 341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.802 46.400 25.829 1.00 120.90	65			LEU C						
341 N SER C 46 8.458 48.758 25.915 1.00 104.59 342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.802 46.400 25.829 1.00 120.90						9.084				
342 CA SER C 46 7.636 47.784 25.206 1.00 104.59 343 CB SER C 46 7.802 46.400 25.829 1.00 120.90									1.00	
70 344 00 650 0 46 7000 25.025 1.00 120.90									1.00	104.59
7.052 45.423 25.111 1.00 120.90	70									
			Ju	JLN U	70	7.002	40,423	25.111	1.00	120.90

	345 346	C O	SER C	46 46	6.194 5.867	48.226 49.072	25.309 26.127	1.00 1.00	104.59 104.59
	347 348	N	GLU C	47	5.320	47.643	24.495	1.00	161.06
5	349	CA CB	GLU C	47 47	3.919	48.057	24.551	1.00	161.06
	350	CG	GLU C	47	3.295 4.218	48.100 48.523	23.152	1.00	249.30
	351	CD	GLU C	47	3.700	48,108	22.010 20.617	1.00 1.00	249.30
	352	OE1	GLU C	47	4.006	46.969	20.155	1.00	249.30 249.30
10	353	OE2	GLU C	47	2.988	48.918	19.972	1.00	249.30
10	354 355	C	GLU C	47	3.070	47.171	25.505	1.00	161.06
	356	N	GLU C	47 48	1.875 3.655	47.409 46.147	25.648	1.00	161.06
	357	CA	GLU C	48	2.859	45.337	26.142 27.077	1.00 1.00	104.22
	358	CB	GLU C	48	3.427	43.913	27.044	1.00	104.22 144.62
15	359	CG	GLU C	48	2.742	43.070	28.349	1.00	144.62
	360 361	CD OE1	GLU C	48	1.288	42.704	28.064	1.00	144.62
	362	OE2	GLU C	48 48	1.034	41.897	27.140	1.00	144.62
	363	c	GLU C	48	0.396 2. 82 9	43.221 46.060	28.775 28.424	1.00	144.62
20	364	Ö	GLU C	48	3.708	46 368	28.724	1.00 1.00	104.22
	365	N	THR C	49	1.813	40.771	29.229	1.00	104. <u>22</u> 87.76
	366	CA	THR C	49	1.677	46.399	30.529	1.00	87.76
	367 368	CB	THR C	49	0.505	47.406	30.547	1.00	167.47
25	369	OG1 CG2	THR C THR C	49	-0.713	46.751	30.168	1.00	167.47
	370	C	THR C	49 49	0.788 1.461	48.5≾6 45.342	29.576	1.00	167.47
	371	ŏ	THR C	49	1.832	45.537	31.601 32.751	1.00 1.00	87.76
	372	N	ASN C	50	0.872	44.210	31.227	1.00	87.76 92.41
30	373	CA	ASN C	50	0.637	43.123	32.180	1.00	92.41
30	374 375	CB	ASN C	50	0.006	41.921	31.455	1.00	211.05
	376	CG OD1	ASN C ASN C	50	-0.583	40.901	32.411	1.00	211.05
	377	ND2	ASN C	50 50	-0.245 -1.449	40.896 40.025	33.593	1.00	211.05
	378	C	ASN C	50	2.006	40.025 42.743	31.907 32.772	1.00 1.00	211.05
35	379	0	ASN C	50	3.035	42.908	32.125	1.00	92.41 92.41
	380	N	SER C	51	2.026	42.252	34.005	1.00	91.81
	381 382	CA CB	SER C	51	3.280	41.858	34.640	1.00	91.81
	383	OG	SER C SER C	51 51	3.042	41.518	36.117	1.00	188.83
40	384	č	SER C	51 51	2.293 3.948	40.322 40.661	36.271	1.00	188.83
	385	Ó	SER C	51	5.130	40.414	33.944 34.137	1.00 1.00	91.81
	386	N	SER C	52	3.199	39.919	33.136	1.00	91.81 82.66
	387	CA	SER C	52	3.750	38.764	32.450	1.00	82.66
45	388 389	CB OG	SER C	52	2.862	37.530	32.662	1.00	107.08
73	390	C	SER C SER C	52 52	2.845 3.860	37.147	34.025	1.00	107.08
	391	ŏ	SER C	52 52	2.866	39.064 39.155	30.976 30.271	1.00	82.66
	392	N	LEU C	53	5.089	39.228	30.524	1.00 1.00	82.66 52.71
50	393	CA	LEU C	53	5.386	39.501	29.126	1.00	52.71 52.71
50	394 395	CB	LEU C	53	6.563	40.483	29.036	1.00	59.51
	396	CG CD1	LEU C	53	7.380	40.539	27.742	1.00	59.51
	397	CD2	LEU C	53 53	6.474 8.217	40.524	26.514	1.00	59.51
	398	C	LEU C	53	5.741	41. 79 7 38.215	27.765 28.378	1.00	59.51
55	399	0	LEU C	53	6.880	37.750	28.462	1.00 1.00	52.71 52.71
	400	N	ASN C	54	4.794	37.650	27.631	1.00	78.83
	401 402	CA	ASN C	54	5.073	36.425	26.889	1.00	78.83
	402	CB CG	ASN C ASN C	54	3.777	35.731	26.511	1.00	114.28
60	404	OD1	ASN C	54 54	3.093 3.685	35.117	27.699	1.00	114.28
	405	ND2	ASN C	54	1.842	34.315 35.488	28.415 27.922	1.00	114.28
	406	С	ASN C	54	5.898	36.641	25.629	1.00 1.00	114.28 78.83
	407	0	ASN C	54	5.983	37.745	25.099	1.00	78.83
65	408	N	ILE C	55	6.527	35.566	25.174	1.00	69.41
UJ	40 9 410	CA CB	ILE C	55 55	7.321	35.571	23.962	1.00	69.41
	411	CG2	ILE C	55 55	8.814	35.555	24.270	1.00	55.40
•	412	CG1	ILE C	55	9.596 9.238	35.167 36.952	23.036	1.00	55.40
	413	CD1	ILE C	55	10.730	37.122	24.724 25.012	1.00 1.00	55.40
70	414	С	ILE C	55	6.935	34.320	23.210	1.00	55.40 69.41
									V0.71

	415	0	ILE C	55	· 7.048	33.232	23.744	1.00	00.44
	416	N	VAL C	56	6.442	34.473	21.989	1.00	69.41 107.00
	417	CA	VAL C	56	6.046	33.317	21.199	1.00	107.00
5	418 - 419	CB CG1	VAL C	56	4.721	33.566	20.504	1.00	128.23
,	420	CG2	VAL C VAL C	56 56	4.126 3.772	32,254 34 <i>,2</i> 77	20.058	1.00	128.23
	421	Č	VAL C	56	7.132	33.041	21.453 20.171	1.00 1.00	128.23
	422	0	VAL C	56	8.236	33.546	20.317	1.00	107.00 107.00
10	423	N	ASN C	57	6.837	32.251	19.142	1.00	99.37
10	424	CA	ASN C	57	7.833	31.906	18.123	1.00	99.37
	425 426	CB CG	ASN C ASN C	57	7.201	31.916	16.733	1.00	170.52
	427	OD1	ASN C	57 57	6.217 6.543	30.781 29.617	16.541 16.766	1.00	170.52
	428	ND2	ASN C	57	5.000	31.115	16.127	1.00 1.00	170.52 170.52
15	429	Č	ASN C	57	9.053	32.828	18.157	1.00	99.37
	430 431	0	ASN C	57	9.105	33.850	17.480	1.00	99.37
	432	N CA	ALA C ALA C	58 58	10.033	32.443	18.966	1.00	78.85
	433	CB	ALA C	58	11.241 12.180	33.220 32.478	19.162 20.085	1.00	78.85
20	434	C	ALA C	58	11.951	33.558	17.878	1.00 1.00	109.58 78.85
	435	0	ALA C	58	12.358	32.681	17.139	1.00	78.85
	436 437	N CA	LYS C	59	12.094	34.845	17.610	1.00	66.66
	437 438	CB	LYS C LYS C	59 59	12.812	35.317	16.428	1.00	66.66
25	439	CG	LYS C	59 59	11.988 10.597	36.405 35.939	15.726 15.295	1.00	201.62
	440	CD	LYS C	59	9.751	37. 0 70	14.724	1.00 1.00	201.62 201.62
	441	CE	LYS C	59	8.374	36.569	14.307	1.00	201.62
	442	NZ	LYS C	59	7.518	37.663	13.775	1.00	201.62
30	443 444	C O	LYS C LYS C	59 50	14.146	35.890	16.953	1.00	66.66
50	445	Ň	PHE C	59 60	14.194 15.224	36.455 35.743	18.055	1.00	66.66
	446	CA	PHE C	60	16.515	36.265	16.188 16.616	1.00 1.00	69.57
	447	CB	PHE C	60	17.455	36.314	15.438	1.00	69.57 112.86
35	448	CG	PHE C	60	17.775	34.974	14.896	1.00	112.86
33	449 450	CD1 CD2	PHE C	60	18.097	34.805	13.562	1.00	112.86
	451	· CE1	PHE C	60 60	17.757 18.396	33.867 33.553	15.718	1.00	112.86
	452	CE2	PHE C	60	18.050	32.608	13.046 15.217	1.00 1.00	112.86 112.86
40	453	CZ	PHE C	60	18.372	32.452	13.877	1.00	112.86
40 .	454	C	PHE C	60	16.436	37.644	17.258	1.00	69.57
	455 456	0 N	PHE C GLU C	60	17.213	37.958	18.172	1.00	69.57
	457	CA CA	GLU C	61 61	15.498 15.308	38.466 39.823	16.785 17.303	1.00	114.60
	458	CB	GLU C	61	14.268	40.583	16.482	1.00 1.00	114.60 179.88
45	459	CG	GLU C	61	14.629	40.775	15.025	1.00	179.88
	460	CD	GLU C	61	14.804	39.464	14.296	1.00	179.88
	461 462	OE1 OE2	GLU C	61	13.874	38.631	14.334	1.00	179.88
	463	C	GLU C	61 61	15.871 14.865	39.269 39.831	13.682	1.00	179.88
50	464	ŏ	GLU C	61	15.064	40.828	18.757 19.451	1.00 1.00	114.60
	465	N	ASP C	62	14.251	38.737	19.214	1.00	114.60 61.26
	466	CA	ASP C	62	13.807	38.654	20.605	1.00	61.26
	467 468	CB CG	ASP C	62	12.884	37.457	20.801	1.00	109.78
55	469	OD1	ASP C ASP C	62 62	11.707 11.182	37.472 38.574	19.842	1.00	109.78
	470	OD2	ASP C	62	11.296	36.385	19.564 19.374	1.00 1.00	109.78
	471	. C	ASP C	62	15.018	38.559	21.542	1.00	109.78 61.26
	472	0	ASP C	62	14.915	38.859	22.726	1.00	61.26
60	473 474	N CA	SER C	63	16.166	38.159	20.999	1.00	49.60
OO.	475	CA CB	SER C SER C	63	17.390	38.050	21.776	1.00	49.60
	476	og Og	SER C	63 63	18.539 18.360	37.599 36.265	20.873 20.405	1.00	59.31
	477	Č	SER C	63	17.669	39.432	20.405 22.294	1.00 1.00	59.31 49.60
C F	478	0	SER C	63	17.647	40.359	21.520	1.00	49.60
65	479	N CA	GLY C	64	17.918	39.595	23.583	1.00	66.63
	480 481	CA C	GLY C	64	18.192	40.936	24.070	1.00	66.63
	482	ŏ	GLY C	64 64	18.223 18.210	41.119 40.154	25.579 26.220	1.00	66.63
-	483	Ň	GLU C	65	18.288	42.371	26.339 26.018	1.00 1.00	68.63 55.08
70	484	CA	GLU C	65	18.306	42.725	27.440	1.00	55.08
									30.00

	485 486	CB	GLU C	65 65	- 19.339 19.349	43.828 44.480	27.632 28.979	1.00 1.00	156.42 156.42
	487	CD	GLU C	65	20.163	45.756	28.978	1.00	156.42
5	488 489	OE1 OE2	GLU C	65 65	19.785	46.700	28.254	1.00	156.42
3	490	C	GLU C	65 65	21.183 16.899	45.817 43.218	29.696	1.00	156.42
	491	ŏ	GLU C	65	16.346	44.123	27.844 27.213	1.00	55.08
	492	Ň	TYR C	66	16.307	42.625	28.871	1.00 1.00	55.08
	493	CA	TYR C	66	14.981	43.056	29.291	1.00	61.99 61.99
10	494	CB	TYR C	66	14.013	41.901	29.181	1.00	58.17
	495	CG	TYR C	66	13.740	41.415	27.806	1.00	58.17
	496 497	CD1 CE1	TYR C TYR C	66	14.658	40.634	27.133	1.00	58.17
	498	CD2	TYR C TYR C	66 66	14.365 12.520	40.112	25.886	1.00	58.17
15	499	CE2	TYR C	66	12.520	41.681 41.170	27.198 25.953	1.00	58.17
	500	CZ	TYR C	66	13.134	40.379	25.300	1.00 1.00	58.17 58.17
	501	ОН	TYR C	66	12.786	39.826	24.081	1.00	58.17
	502	Ç	TYR C	66	14.950	43.525	30.746	1.00	61.99
20	503	o O	TYR C	66	15.850	43.192	31.522	1.00	61.99
20	504 505	N CA	LYS C LYS C	67	13.899	44.254	31.132	1.00	84.17
	506	CB	LYS C LYS C	67 67	13.751	44.703 45.766	32.516	1.00	84.17
	507	ČĠ	LYS C	67	14.789 14.858	45.766 46.850	32.837 31.807	1.00 1.00	116.03
	508	∢ CD	LYS C	67	15.986	47.803	32.118	1.00	116.03 116.03
25	509	CE	LYS C	67	16.177	48.787	30.983	1.00	116.03
	510	NZ	LYS C	67	17.324	49.693	31.252	1.00	116.03
	511	C	LYS C	67	12.369	45.249	32.762	1.00	84.17
	512 513	0 N	LYS C CYS C	67	11.696	45.655	31.819	1.00	84.17
30	514	CA	CYS C CYS C	68 68	11.933 10.624	45.229 45.780	34.020	1.00	81.35
-	515	Č	CYS C	68	10.749	46.788	34.350 35.467	1.00 1.00	81.35
	516	ō	CYS C	68	11.761	46.811	36.145	1.00	81.35 81.35
,	517	СВ	CYS C	68	9.619	44.672	34.717	1.00	117.98
25	518	ŞG	CYS C	68	9.997	43.610	36.128	1.00	117.98
35	519	N OA	GLN C	69	9.734	47.628	35.627	1.00	106.08
	520 521	CA CB	GLN C GLN C	69	9.722	48.638	36.664	1.00	106.08
	522	CG	GLN C	69 69	10.471 10.166	49.900 51.173	36.188 36.978	1.00	124.18
	523	CD	GLN C	69	10.841	52.407	36.397	1.00 1.00	124.18 124.18
40	524	OE1	GLN C	69	10.720	52.687	35.205	1.00	124.18
	525	NE2	GLN C	69	11.542	53.160	37.244	1.00	124.18
	526	C	GLN C	69	8.265	48.974	36.930	1.00	106.08
	527 528	0 N	GLN C	69	7.416	48.787	36.054	1.00	106.08
45	529	CA	HIS C HIS C	70 70	7.967 6.609	49.457 49.830	38.131	1.00	181.43
	530	CB	HIS C	70	6.177	49.107	38.469 39.764	1.00 1.00	181.43
	531	CG	HIS C	70	6.062	47.635	39.606	1.00	144.62 144.62
	532	CD2	HIS C	70	6.901	46.634	39.977	1.00	144.62
50	533	ND1	HIS C	70	4.972	47.041	39.030	1.00	144.62
30	534 535	CE1	HIS C	70	5.121	45.722	39.060	1.00	144.62
	536	NE2 C	HIS C HIS C	70 70	6.283 6.421	45.464	39.631	1.00	144.62
	537	ŏ	HIS C	70 70	7.299	51.335 52.112	38.609 38.268	1.00	181.43
	538	Ň	GLN C	71	5.254	51.714	39.108	1.00 1.00	181.43 249.25
55	539	CA	GLN C	71	4.925	53.108	39.290	1.00	249.25
	540	CB	GLN C	71	3.550	53.209	39.950	1.00	249.45
	541	ca	GLN C	71	2.717	54.409	39.544	1.00	249.45
	542 543	CD OE1	GLN C	71	2.659	54.624	38.057	1.00	249.45
60	544	NE2	GLN C GLN C	71 71	1.970 3.360	53.886 55. 62 6	37.367	1.00	249.45
	545	C	GLN C	71	5.988	53.876	37.553 40.093	1.00 1.00	249.45
	546	Ö	GLN C	71	6.510	54.891	39.634	1.00	249.25 249.25
	547	Ņ	GLN C	72	6.321	53.366	41.276	1.00	190.92
4 E	548	CA	GLN C	72	7.312	54.001	42.145	1.00	190.92
65	549	CB	GLN C	72	6.639	54.552	43.406	1.00	249.44
	550 551	CG CD	GLN C	72	7.556	55.342	44.333	1.00	249.44
	552	OE1	GLN C GLN C	72 72	6.833 5.871	55.900 56.656	45.543	1.00	249.44
	553	NE2	GLN C	72	7.296	56.656 55.530	45.411 46.734	1.00	249.44
70	554	c c	GLN C	72	8.427	53.034	46.734 42. 54 6	1.00 1.00	249.44 190.92
					·		72.070	1.00	180.82

	555	0	GLN C	72	- 8.660	52,788	43.734	1.00	100.00
	556	N.	VAL C	73	9.118	52.481	41.556	1.00	190.92 211.52
	557 558	CA CB	VAL C VAL C	73	10.183	51.531	41.836	1.00	211.52
5	559	CG1	VAL C	73 73	9.649 10.667	50.092 49.148	41.803 42.403	1.00	215.95
	560	CG2	VAL C	73	8.338	50.011	42.403 42.539	1.00 1.00	215.95
	561	C	VAL C	73	11.297	51.639	40.816	1.00	215.95 211.52
	562 563	0 N	VAL C ASN C	73	11.053	51.942	39.649	1.00	211.52
10	564	ČA	ASN C	74 74	12.525 13.656	51.391 51.454	41.256 40.349	1.00	137.61
	565	CB	ASN C	74	14.950	51.650	41.136	1.00 1.00	137.61 154.43
	566	CG	ASN C	74	14.895	52.860	42.037	1.00	154.43
	567 568	OD1 ND2	ASN C ASN C	74 74	14.408	53.920	41.631	1.00	154.43
15	569	C	ASN C	74	15.401 13.708	52.711 50.169	43.259 39.523	1.00 1.00	154.43
	570	0	ASN C	74	13.641	49.062	40.063	1.00	137.61 137.61
	571	N	GLU C	75	13.807	50.341	38.205	1.00	102.99
	572 573	CA CB	GLU C	75 75	13.862 14.305	49.236	37.248	1.00	102.99
20	574	CG	GLU C	75 75	15.294	49.764 50.916	35.881 35.952	1.00 1.00	231.35
	575	CD	GLU C	75	15.534	51.559	34.601	1.00	. 231.35 231.35
	576	OE1	GLU C	75	14.547	51.970	33.952	1.00	231.35
	577 578	OE2 C	GLU C	75 75	16.710	51.657	34.190	1.00	231.35
25	579	ŏ	GLU C	75 75	14.749 15.794	48.080 48.281	37.693	1.00	102.99
	580	N	SER C	76	14.305	46.868	38.296 37.383	1.00 1.00	102.99 85.19
	581	CA	SER C	76	14.987	45.629	37.747	1.00	85.19
	582 583	CB OG	SER C	76	14.101	44.446	37.402	1.00	104.06
30	584	C	SER C SER C	76 76	13.920 16.308	44.371 45.424	35.992	1.00	104.06
	585	Ŏ	SER C	76	16.560	46,020	37.044 35.998	1.00 1.00	85.19 85.19
	586	N	GLU C	77	17.140	44.553	37.612	1.00	76.77
	587 588	CA CB	GLU C	77	18.444	44.238	37.023	1.00	76.77
35	589	CG	GLU C	77 77	19.263 19.643	43.355 44.039	37.962	1.00	228.57
	590	CD	GLU Č	77	20.577	45.228	39.268 39.070	1.00 1.00	228.57 228.57
	591	OE1	GLU C	77	20.709	45.703	37.921	1.00	228.57 228.57
	592 593	OE2	GLU C	77	21.172	45.695	40.068	1.00	228.57
40	593 594	C	GLU C	77 77	18.178 17.573	43.498	35.728	1.00	76.77
	595	Ň	PRO C	78	18.600	42.420 44.080	35.746 34.585	1.00 1.00	76.77
	596	CD	PRO C	78	19.176	45.434	34.463	1.00	81.92 75.82
	597 598	CA CB	PRO C	78	18.417	43.503	33.255	1.00	81.92
45	599	CG	PRO C PRO C	78 78	19.357 19.130	44.328	32.394	1.00	75.82
	600	č	PRO C	78	18.717	45.681 42.029	32.940 33.190	1.00 1.00	75.82
	601	0	PRO C	78	19.475	41.508	34.000	1.00	81.92 81.92
	602 603	N	VAL C	79	18.094	41.357	32.233	1.00	71.44
50	604	CA CB	VAL C VAL C	79 79	18.300	39.938	32.036	1.00	71.44
	605	CG1	VAL. C	79	17.121 17.199	39.139 37.717	32.538 32.029	1.00 1.00	74.89
	606	CG2	VAL C	79	17.131	39.154	34.047	1.00	74.89 74.89
	607	C	VAL C	79	18.454	39.707	30.552	1.00	71.44
55	608 609	O N	VAL C TYR C	79	17.646	40.184	29.748	1.00	71.44
	610	CA	TYR C	80 80	19.502 19.710	38.989 38.728	30.179 28.773	1.00	69.00
	611	СВ	TYR C	80	21.184	38.7-7	28.406	1.00 1.00	69.00 132.22
	612	CG	TYR C	80	21.361	38.905	26.921	1.00	132.22
60	613 614	CD1 CE1	TYR C Tyr C	80	20.962	40.075	26.284	1.00	132.22
•	615	CD2	TYR C	80 80	21.102 21.902	40.236 37.891	24.923	1.00	132.22
	616	CE2	TYR C	80	22.039	38.046	26.143 24.754	1.00 1.00	132.22 132.22
	617	CZ	TYR C	80	21.636	39.228	24.163	1.00	132.22
65	618 619	он	TYR C	80	21.777	39.415	22.807	1.00	132.22
5 5	620	C	TYR C TYR C	80 80	19.150 19.295	37.401	28.300	1.00	69.00
	621	Ň	LEU C	81	18.534	36.380 37.423	28.939 27.141	1.00 1.00	69.00
	622	CA	LEU C	81	17.988	36.232	26.557	1.00	61.97 61.97
70	623 624	CB CC	LEU C	81	16.501	36.449	26.351	1.00	56.21
, 0	UZ4	CG	LEU C	81	15.878	35.304	25.589	1.00	56.21

	625 626	CD1 CD2	LEU C	81	.16.017	34.060	26.431	1.00	56.21
	627	C	LEU C	81 81	14.424	35.608	25.294	1.00	58.21
	628	ŏ	LEU C	81	18.700 18.814	36.019 36.949	25.213 24 <i>.</i> 423	1.00	61.97
5	629	Ň	GLU C	82	19.191	34.816	24.948	1.00 1.00	61.97
	630	CA	GLU C	82	19.855	34.581	23.674	1.00	70.61 70.61
	631	CB	GLU C	82	21.326	34.242	23.882	1.00	114.25
	632	CG	GLU C	82	22.179	34.569	22.675	1.00	114.25
10	633 634	CD OE1	GLU C	82	23.657	34.256	22.884	1.00	114.25
10	635	OE2	GLU C GLU C	82 82	24.149	34.456	24.020	1.00	114.25
	636	C	GLU C	82	24.331 19.172	33.827 33.457	21.913 22.896	1.00 1.00	114.25
	637	Ŏ	GLU C	82	18.913	32.381	23.440	1.00	70.61
	638	N	VAL C	83	18.886	33.706	21.622	1.00	70.61 70.46
15	639	CA	VAL C	83	18.225	32.717	20.795	1.00	70.46
	640	CB	VAL C	83	17.114	33.346	20.004	1.00	68.26
	641 642	CG1 CG2	VAL C VAL C	83	16.531	32.318	19.057	1.00	68.26
	643	C	VAL C VAL C	83 83	16.045 19.156	33.848	20.941	1.00	68.26
20	644	ŏ	VAL C	83	19.156	32.014 32.663	19.825 19.157	1.00	70.46
	645	Ň	PHE C	84	19.031	30.694	19.718	1.00 1.00	70.46 54.26
	646	CA	PHE C	84	19.913	29.944	18.845	1.00	54.26
	647	CB	PHE C	84	20.793	28.988	19.650	1.00	65.02
25	648	CG	PHE C	84	21.645	29.643	20.638	1.00	65.02
23	649 650	CD1	PHE C	84	21.104	30.128	21.788	1.00	65.02
	651	CD2 CE1	PHE C PHE C	84	22.996	29.767	20.426	1.00	65.02
	652	CE2	PHE C	84 84	21.897 23.811	30.746 30.384	22.733	1.00	65.02
	653	CZ	PHE C	84	23.262	30.872	21.359 22.519	1.00 1.00	65.02
30	654	С	PHE C	84	19.247	29.092	17.790	1.00	65.02 54.26
	655	0	PHE C	84	18.045	28.781	17.861	1.00	54.26
	656	N	SER C	85	20.101	28.686	16.849	1.00	85.79
	657 658	CA	SER C	85	19.768	27.807	15.750	1.00	85.79
35	659	CB OG	SER C SER C	85 85	19.683	28.583	14.435	1.00	134.11
-	660	Č	SER C	85	19.375 20.951	27.719 26.860	13.355 15.700	1.00	134.11
	661	ŏ	SER C	8 5	22.063	27.274	15.360	1.00 1.00	85.79 85.79
	662	N	ASP C	86	20.731	25.607	16.083	1.00	52.64
40	663	CA	ASP C	86	21.798	24.604	16.049	1.00	52.64
40	664	CB	ASP C	86	22.912	24.984	17.015	1.00	115.87
	665 666	CG OD1	ASP C ASP C	86	24.265	24.581	16.504	1.00	115.87
	667	OD2	ASP C	86 86	24.448 25.144	23.384 25.459	16.194	1.00	115.87
	668	C	ASP C	86	21.199	23.235	16.411 16.420	1.00 1.00	115.87
45	669	0	ASP C	86	20.051	23.168	16.879	1.00	52.64 52.64
	670	N	TRP C	87	21.944	22.146	16.202	1.00	58.25
	671	CA	TRP C	87	21.424	20.809	16.522	1.00	58.25
	672 673	CB CG	TRP C	87	22.372	19.723	16.049	1.00	247.83
50	674	CD2	TRP C	87 87	22.083 22.700	19.354	14.675	1.00	247.83
-	675	CE2	TRP C	87	22.700	19.899 19.344	13.518 12.404	1.00 1.00	247.83
	676	CE3	TRP C	87	23.742	20.812	13.311	1.00	247.83 247.83
	677	CD1	TRP C	87	21.106	18.504	14.235	1.00	247.83
e e	678	NE1	IRP C	87	21.082	18.496	12.867	1.00	247.83
5 5	679	CZ2	TRP C	87	22.418	19.660	11.113	1.00	247.83
	680 681	CZ3 CH2	TRP C	87	24.098	21.132	12.023	1.00	247.83
	682	CH2 C	TRP C	87 87	23.444 21.220	ے0.552 20.650	10.944	1.00	247.83
	683	ŏ	TRP C	87	20.141	20.656 20.260	18.009	1.00	58.25
60	684	Ň	LEU C	88	22.264	20.985	18.463 18.760	1.00 1.00	58.25 79.45
	685	CA	LEU C	88	22.230	20.887	20.197	1.00	79.45 79.45
	686	СВ	LEU C	88	23.225	19.845	20.659	1.00	5 7.9 7
	687	CG	LEU C	88	22.896	18.431	20.245	1.00	57.97
65	688 689	CD1 CD2	LEU C	88	23.876	17.490	20.880	1.00	57.97
55	690	CD2	LEU C	88 88	21.495	18.114	20.693	1.00	57.97
	691	ŏ	LEU C	88	22.558 23.432	22.194 22.940	20.870	1.00	79.45
	692	Ň	LEU C	89	21.872	22. 94 0 22.451	20.419 21.976	1.00 1.00	79.45
70	693	CA	LEU C	89	22.097	23.669	22.732	1.00	57.52 57.52
70	694	СВ	LEU C	89	20.919	24.616	22.578	1.00	59.32

	695 696	CG CD1		C 89		25.884 26.439	23.373 23.134		59.32
	697	CD2		C 89		26.861	22.941	1.00	59.32
_	698	C .	LEU	C 89		23.316	24.184		59.32 57.52
5	699	0	LEU		21.432	22.577	24.697		57.52 57.52
	700	N		C 90		23.8 15	24.846	1.00	64.90
	701	CA		C 90		23.521	26.267		64.90
	702 703	CB CG	LEU			23.512	26.638		46.55
10	703	CD1	LEU			23.312 21.955	28.119		46.55
	705	CD2	LEU			23.409	28.491 28.423	1.00 1.00	46.55
	706	С	LEU			24.591	27.083		46.55 64.90
	707	0	LEU		23.167	25.754	27.032		64.90
16	708	N	GLN			24.208	27.852		56.08
15	709	CA CB	GLN			25.187	28.650		56.08
	710 711	CG	GLN GLN		_	24.944	28.517		49.57
	712	CD	GLN			25.036 25.013	27.094 26.979		49.57
	713	OE1	GLN			23.977	27. 2 45	1.00 1.00	49.57 49.57
20	714	NE2	GLN			26.167	26.601	1.00	49.57
	715	Ç	GLN		21.440	25.146	30.103	1.00	56.08
	716	0	GLN			24.066	30.638	1.00	56.08
	717 718	N CA		C 92		26.309	30.752	1.00	47.15
25	719	· CA CB	ALA ALA	C 92 C 92		26.335	32.166	1.00	47.15
	720	C		C 92 C 92		26.962 27.102	32.345 32.955	1.00	42.48
	721	ŏ		C 92		28.102	32.474	1.00 1.00	47.15
	722	N	SER			26.620	34.151	1.00	47.15 67.10
20	723	CA	SER			27.289	35.013	1.00	67.10
30	724	СВ	SER			26.625	36.392	1.00	100.79
	725	og Og	SER			26.434	36.965	1.00	100.79
	726 727	C O	SER SER	_		28.705	35.137	1.00	67.10
	728	Ň	ALA			29.632 28.868	34.692 35.704	1.00	67.10
35	729	CA		C 94	21.818	30.179	35.875	1.00 1.00	57.34 57.34
	730	СВ	ALA		21.716	30.609	37.326	1.00	92.07
	731	C		C 94	23.279	30.072	35.462	1.00	57.34
	732	0	ALA		23.912	29.048	35.694	1.00	57.34
40	733 734	N CA	GLU (C 95		31.123	34.860	1.00	69.09
40	735	CB	GLU		25.212 25.403	31.088 31.994	34.419	1.00	69.09
	736	ČĞ	GLU			31.618	33.214 32.048	1.00 1.00	142.79 142.79
	737	CD	GLU		24.954	32.288	30.759	1.00	142.79
45	738	OE1	GLU (24.268	32.084	29.733	1.00	142.79
45	739	OE2	GLU (25.976	33.013	30.767	1.00	142.79
	740 741	C O	GLU (26.232	31.459	35.494	1.00	69.09
	742	N	GLU VAL		27.435 25.765	31.238	35.316	1.00	69.09
	743	CA		C 96 C 96	26.640	32.041 32.419	36.598 37.713	1.00 1.00	86.41
50	744	CB		C 96	26.922	33.903	37.702	1.00	86.41 74.25
	745	CG1		C 96	28.119	34,207	38.587	1.00	74.25 74.25
	746	CG2		C 96	27.176	34.357	36.277	1.00	74.25
	747	C	VAL		25.910	32.052	38.990	1.00	86.41
55	748 749	0 N	VAL.			32.348	39.135	1.00	86.41
55	750	CA	VAL (C 97 C 97	26.610 25.953	31.434 30.955	39.931	1.00	73.13
	751	CB	VAL	C 97	25.697	29.456	41.142 41.001	1.00 1.00	73.13
	752	CG1	VAL	C 97		28.999	42.037	1.00	48.19 48.19
	753	CG2	VAL			29.146	39.634	1.00	48.19
60	754	C	VAL		26.715	31.125	42.448	1.00	73.13
	755 756	0	VAL		27.924	30.893	42.513	1.00	73.13
	756 757	N CA	MET (25.999	31.490	43.503	1.00	70.97
	757 758	CB	MET		26.612 25.638	31.622	44.828	1.00	70.97
65	759	ČG	MET		25.295	32.331 33.728	45.763 45.318	1.00 1.00	151.84
	760	SD	MET		26.581	34.857	45.790	1.00	151.84 151.84
	761	CE	MET	C 98	26.247	34.962	47.553	1.00	151.84
	762	C	MET		26.930	30.228	45.390	1.00	70.97
70	763 764	0	MET	_		29.335	45.348	1.00	70.97
, 0	7 UT	N	GLU (C 99	28.130	30.037	45.923	1.00	61.59

		•	-						
	765 768	CA CB	GLU C	99	28.508	28.740	48.475	1.00	61.59
	767	CG	GLU C	99	29.762 30.525	28.874	47.339	1.00	200.85
	768	CD	GLU C	99	30.525 31.581	27.574	47.520	1.00	200.85
5	769	OE1	GLU C	99	32.197	27.657 28.724	48.623 48.761	1.00	200.85
	770	OE2	GLU C	99	31.746	26.651	49.342	1.00 1.00	200.85
	771	С	GLU C	99	27.354	28.221	47.325	1.00	200.85 61.59
	772	0	GLU C	99	26.851	28.934	48.184	1.00	61.59
10	773	N	GLY C	100	26.901	27.000	47.076	1.00	69.94
10	774	CA	GLY C	100	25.819	26.456	47.876	1.00	69.94
	775 776	CO	GLY C	100	24.468	26.355	47.191	1.00	69.94
	776 777	N	GLY C GLN C	100	23.600	25.591	47.657	1.00	69.94
	778	ĞA	GLN C	101 101	24.266 22.990	27.111 27.083	46.105	1.00	57.42
15	779	СВ	GLN C	101	22.778	28.399	45.370 44.634	1.00 1.00	57.42
	730	CG	GLN C	101	22.627	29.570	45.551	1.00	124.38 124.38
	781	CD	GLN C	101	21.628	29.295	46.641	1.00	124.38
	782	OE1	GLN C	101	21.911	28.587	47.605	1.00	124.38
20	783	NE2	GLN C	101	20.438	29.839	46.485	1.00	124.38
20	784 785	C O	GLN C	101	22.854	25.918	44.369	1.00	57.42
	786	N	GLN C PRO C	101 102	23.834 21.627	25.2)	44.031	1.00	57.42
	787	CD	PRO C	102	20.356	25.663 26.358	43.893 44.165	1.00	52.71
	788	CA.	PRO C	102	21.438	24.573	42.942	1.00 1.00	80.58
25	789	CB	PRO C	102	19.957	24.318	43.044	1.00	52.71 80.58
	790	CG	PRO C	102	19.422	25.709	43.171	1.00	80.58
	791	Ç	PRO C	102	21.870	25.005	41.531	1.00	52.71
	792	. 0	PRO C	102	21.853	26.203	41.189	1.00	52.71
30	793 794	N CA	LEU C LEU C	103	22.242	24.033	40.705	1.00	64.68
50	795	CB	LEU C	103 103	22.661 24.172	24.323 24.347	39.343	1.00	64.68
	796	CG	LEU C	103	24.605	24.608	39.273 37.838	1.00 1.00	81.00
	797	CD1	LEU C	103	24.136	25.987	37.435	1.00	81.00 81.00
25	798	CD2	LEU C	103	26.113	24.486	37.718	1.00	81.00
35	799	Ç	LEU C	103	22.147	23.244	38.403	1.00	64.68
	800	0 N	LEU C	103	22.418	22.063	38.642	1.00	64.68
	801 802	CA	PHE C	104	21.409	23.616	37.355	1.00	64.85
	803	CB	PHE C	104 104	20.923 19.392	22.599 22.530	36.423	1.00	64.85
40	804	ČĠ	PHE C	104	18.787	22.248	36.418 37.758	1.00 1.00	111.94
	805	CD1	PHE C	104	18.694	23.250	38.710	1.00	111.94 111.94
	806	CD2	PHE C	104	18.300	20.980	38.068	1.00	111.94
	807	CE1	PHE C	104	18.128	23.000	39.962	1.00	111.94
45	808 809	CE2 CZ	PHE C	104	17.731	20.717	39.320	1.00	111.94
70	810	C C	PHE C PHE C	104	17.644	21.732	40.268	1.00	111.94
	811	. ŏ	PHE C	104 104	21.410 21.254	22.829 23.915	34.993	1.00	64.85
	812	N	LEU C	105	22.009	21.817	34.462 34.371	1.00 1.00	64.85
	813	CA	LEU C	105	22.469	21.933	32.983	1.00	49.42 49.42
50	814	CB	LEU C	105	23.928	21.502	32.848	1.00	35.01
	815	CG	LEU C	105	24.870	22.289	33.757	1.00	35.01
	816	CD1	LEU C	105	26.346	21.971	33.451	1.00	35.01
	817 818	CD2 C	LEU C	105	24.579	23.735	33.535	1.00	35.01
55	819	ŏ	LEU C	105 105	21.603 21.225	21.000	32.181	1.00	49.42
	820	Ň	ARG C	106	21.290	19.954 21.353	32.679 30.946	1.00	49.42
	821	CA	ARG C	106	20.438	20.487	30.155	1.00 1.00	67.77 67.77
	822	CB	AHG C	108	19.027	21.043	30.194	1.00	104.09
60	823	CG	ARG C	106	18.056	20.302	29.334	1.00	104.09
60	824	CD	ARG C	106	16.745	21.071	29.217	1.00	104.09
	825 826	NE C7	ARG C	106	15.814	20.401	28.316	1.00	104.09
	827	CZ NH1	ARG C ARG C	106	14.812	21.002	27.694	1.00	104.09
	828	NH2	ARG C	106 106	14.616 14.023	22.292 20.314	27.879	1.00	104.09
65	829	C	ARG C	106	20.911	20.314	26.879 28.710	1.00	104.09
	830	0	ARG C	106	21.063	21.431	28.053	1.00 1.00	67.77 67.77
	831	Ņ	CYS C	107	21.160	19.179	28.205	1.00	64.22
	832	ÇA	CYS C	107	21.599	19.074	26.819	1.00	64.22
70	833	C	CYS C	107	20.320	19.044	26.063	1.00	64.22
70	834	0	CYS C	107	19.579	18.067	26.143	1.00	64.22

	. 8∟	CB SG	CYS C	107 107	-22.396 23.369	17.808 17.892	26.547 24.999	1.00	74.81
	37	Ň	HIS C	108	20.054	20,132	25.351	1.00	74.81
	<i>1</i> 38	CA	HIS C	108	18.815	20.288	24.593	1.00 1.00	62.02
	.139	CB	HIS C	108	18.257	21.669	24.859	1.00	62.02 73.41
	. 40 .41	CG	HIS C	108	16.893	21.884	24.302	1.00	73.41 73.41
	942	CD2	HIS C	108	16,409	22.839	23.479	1.00	73.41
	843	ND1 CE1	HIS C	108 108	15.821	21.093	24.648	1.00	73.41
	844	NE2	HIS C	108	14.731 15.061	21.558	24.067	1.00	73.41
	845	C	HIS C	108	18.925	22.618 20.085	23.353 23.089	1.00	73.41
	846	Ó	HIS C	108	19.750	20.724	22.412	1.00 1.00	62.02 62.02
	847	Ŋ	GLY C	109	18.066	19.207	22.578	1.00	82.12
15	848 849	CA	GLY C	109	18.075	18.907	21.161	1.00	82.12
13	850	C	GLY C	109	17.196	19.859	20.396	1.00	82.12
	851	Ŋ	GLY C TRP C	109 110	16.281 17.473	20.439	20.963	1.00	82.12
	852	ĈA	TRP C	110	16.691	20.020 20.916	19.107	1.00	66.53
00	853	CB	TRP C	110	17.327	21.057	18.282 16.911	1.00 1.00	66.53
20	854	CG	TRP C	110	16.487	21.825	15.969	1.00	113.55 113.55
	855 856	CD2	TRP C	110	16.565	23.226	15.701	1.00	113.55
	857	CE2 CE3	TRP C	110	15.552	23.532	14.769	1.00	113.55
_	858	CD1	TRP C TRP C	110	17.401	24.260	16.157	1.00	113.55
25	859	NE1	TRP C	110 110	15.460 14.892	21.348 22.364	15.216	1.00	113.55
	860	CZ2	TRP C	110	15.345	24.831	14.490 14.280	1.00 1.00	113.55
	861	CZ3	TRP C	110	17.193	25.561	15.668	1.00	113.55
	862 863	CH2	TRP C	110	16.171	25.829	14.742	1.00	113.55 113.55
30	864	C	TRP C	110	15.284	20.383	18.160	1.00	66.53
	865	Ň	TRP C ARG C	116 111	15.060	19.188	18.276	1.00	66.53
	866	ČA	ARG C	111	14.334 12.928	21.285	17.951	1.00	82.69
•	867	CB	ARG C	111	12.677	20.924 20.368	17.807 16.432	1.00 1.00	82.69
35	868	CG	ARG C	111	12.367	21.439	15.493	1.00	249.07 249.07
33	869 870	CD	ARG C	111	11.908	20.831	14.270	1.00	249.07
	871	NE CZ	ARG C	111	10.787	21.587	13.769	1.00	249.07
	872	NH1	ARG C ARG C	111 111	9.568	21.660	14.334	1.00	249.07
40	873	NH2	ARG C	111	9.309 8.601	20.994 22.346	15.438	1.00	249.07
40	874	Ç	ARG C	111	12.433	19.928	13.736 18.828	1.00 1.00	249.07
	875	0	ARG C	111	11.471	19.213	18.595	1.00	82.69 82.69
	876 877	N ∙CA	ASN C	112	13.119	19.872	19.953	1.00	79.91
	878	CB	ASN C ASN C	112	12.756	18.976	21.027	1.00	79.91
45	879	ČĠ	ASN C	112 112	11.354 11.152	19.288.	21.540	1.00	134.30
	880	OD1	ASN C	112	11.850	18.815 17.902	22.957	1.00	134.30
	881	ND2	ASN C	112	10.194	19.424	23.427 23.653	1.00 1.00	134.30
	882	C	ASN C	112	12.833	17.513	20.651	1.00	134.30 79.91
50	883 884	O N	ASN C TRP C	112	12.172	16.683	21.270	1.00	79.91 79.91
-	885	ČA	TRP C TRP C	113	13.637	17.180	19.650	1.00	91.68
	886	CB	TRP C	113 113	13.771 14.648	15.780	19.287	1.00	91.68
	887	CG	TRP C	113	13.958	15.601 15.923	18.062	1.00	105.58
55	888	CD2	TRP C	113	14.528	16.557	16.805 15.662	1.00	105.58
23	889 890	CE2	TRP C	113	13,524	16.609	14.670	1.00 1.00	105.58 105.58
	891	CE3 CD1	TRP C	113	15.803	17.083	15.373	1.00	105,58
	892	NE1	TRP C TRP C	113 110	12.660 12.393	15.629	16.478	1.00	105.58
	893	CZ2	TRP C	113	13.750	16.038 17.164	15.194	1.00	105.58
60	894	CZ3	TRP C	113	16.030	17.637	13.413 14.119	1.00	105.58
	895	CH5	TRP C	113	15.005	17.676	13.155	1.00 1.00	105.58
	896	C	TRP C	113	14.393	15.003	20.425	1.00	105.58 91.68
	897 898	0 N	TRP C	113	14.528	15.502	21.543	1.00	91.68
65	899	CA CA	ASP C ASP C	114	14.780	13.770	20.133	1.00	96.80
	900	ČB	ASP C	114 114	15.398 14.675	12.926 11.576	21.133	1.00	96.80
	901	, CG	ASP C	114	13.402	11.645	21.213	1.00	249.33
	902	OD1	ASP C	114	13.493	12.001	22.044 23.239	1.00	249.33
70	903	OD2	ASP C	114	12.314	11.344	21.507	1.00 1.00	249.33 249.33
70	904	С	ASP C	114	16.866	12. 72 7	20.813	1.00	96.80
									-0.00

	905	0	ASP C	114	. 17.257	12,561	19.652	1.00	
	906	Ň	VAL C	115	17.678	12.771	21.860	1.00 1.00	96.80
	907	CA	VAL C	115	19.112	12.593	21.728	1.00	71.72 71.72
_	908	СВ	VAL C	115	19.875	13.783	22.274	1.00	77.93
5	909	CG1	VAL C	115	21.344	13.665	21.884	1.00	77.93
	910	CG2	VAL C	115	19.257	15.061	21.751	1.00	77.93
	911 912	c o	VAL C	115	19.535	11.382	22.516	1.00	71.72
	913	N	VAL C TYR C	115 116	18.999 20.502	11.111	23.589	1.00	71.72
10	914	ČA	TYR C	116	20.902	10.653 9.454	21.979 22.644	1.00 1.00	67.55
	915	CB	TYR C	116	20.610	8.219	21.826	1.00	67.55
	916	CG	TYR C	116	19.121	8.010	21.689	1.00	100.42 100.42
	917	CD1	TYR C	116	18.431	8.465	20.572	1.00	100.42
1 5	918	CE1	TYR C	116	17.049	8.284	20.454	1.00	100.42
15	919	CD2	TYR C	116	18.403	7.371	22.690	1.00	100.42
	920 921	CE2 CZ	TYR C	116	17.028	7.185	22.590	1.00	100.42
	922	OH	TYR C TYR C	116	16.352	7.644	21.468	1.00	100.42
	923	C C	TYR C	116 116	14.991 22.514	7.468 9.501	21.357 22.853	1.00	100.42
20	924	ō	TYR C	116	23.187	10.404	22.351	1.00 1.00	67.55
	925	N	LYS C	117	23.040	8.518	23.578	1.00	67.55 124.33
	926	CA	LYS C	117	24.466	8.443	23.848	1.00	124.33
	927	CB	LYS C	117	25.233	7. 94 6	22.617	1.00	168.92
25	928	cg	LYS C	117	25.319	6.439	22.465	1.00	168.92
23	929 930	CD CE	LYS C LYS C	117	26.431	6.073	21.494	1.00	168.92
	931	NZ	LYS C	117 117	27.782	6.589	21.988	1.00	168.92
	932	C	LYS C	117	28.904 24.974	6.284 9.822	21.056 24.229	1.00	168.92
	933	ŏ	LYS C	117	25.904	10.347	23.608	1.00 1.00	124.33 124.33
30	934	N	VAL C	118	24.361	10.406	25.253	1.00	96.88
	935	CA	VAL C	118	24.752	11.731	25.714	1.00	96.88
	936	CB	VAL C	118	23.572	12.432	26.338	1.00	47.91
	937	CG1	VAL C	118	24.036	13.463	27.307	1.00	47.91
35	938 939	CG2 C	VAL C VAL C	118	22.786	13.114	25.264	1.00	47.91
55	940	ŏ	VAL C	118 118	25.914 25.980	11.799 11.030	26.692 27.648	1.00	96.88
	941	Ň	ILE C	119	26.815	12.746	26.455	1.00 1.00	96.88 44.35
	942	CA	ILE C	119	27.968	12.917	27.316	1.00	44.35
40	943	СВ	ILE C	119	29.214	12.377	26.650	1.00	99.63
40	944	CG2	ILE C	119	30.395	12.468	27.585	1.00	99.63
	945 946	CG1	ILE C	119	28.973	10.939	26.239	1.00	99.63
	947	CD1 C	ILE C	119 119	30.044 28.227	10.421	25.309	1.00	99.63
	948	ŏ	ILE C	119	28.466	14.396 15.166	27.618 26.683	1.00	44.35
45	949	Ň	TYR C	120	28.193	14.816	28.889	1.00 1.00	44.35 48.39
	950	CA	TYR C	120	28.478	16.224	29.185	1.00	48.39
	951	CB	TYR C	120	27.803	16.687	30.458	1.00	42.29
	952	CG	TYR C	120	26.322	16.785	30.363	1.00	42.29
50	953 954	CD1 CE1	TYR C	120	25.537	15.697	30.581	1.00	42.29
50	955	CD2	TYR C TYR C	120 120	24.185 25.710	15.775	30.485	1.00	42.29
	956	CE2	TYR C	120	24.340	17.982 18.088	30.035	1.00	42.29
	957	cz	TYR C	120	23.584	16.968	29.924 30.155	1.00	42.29
	958	OH	TYR C	120	22.206	17.007	30.061	1.00 1.00	42.29 42.29
55	959	Ç	TYR C	120	29.962	16.358	29.412	1.00	48.39
	960	0	TYR C	120	30.602	15.447	29.935	1.00	48.39
	961	N	TYR C	121	30.518	17.498	29.053	1.00	53.29
	962 963	CA CB	TYR C	121	31.942	17.700	29.246	1.00	53.29
60	964	CG	TYR C TYR C	121	32.664	17.828	27.887	1.00	75.15
	965	CD1	TYR C	121 121	32.747 31.598	16.569 15.971	27.044 26.525	1.00	75.15
	966	CE1	TYR C	121	31.669	14.849	25.717	1.00 1.00	75.15 75.15
	967	CD2	TYR C	121	33.976	16.002	26.731	1.00	75.15 75.15
4 F	968	CE2	TYR C	121	34.055	14.881	25.921	1.00	75.15
65	969	CZ	TYR C	121	32.895	14.315	25.421	1.00	75.15
	970 971	ŎН	TYR C	121	32.960	13.214	24.613	1.00	75.15
	971 972	C O	TYR C TYR C	121	32.219	18.966	30.056	1.00	53.29
	973	N	LYS C	121 122	31.547	19.984	29.872	1.00	53.29
70	974	ČA	LYS C	122	33.199 33.580	18.908 20.077	30.954	1.00	72.38
				155	J.J.J.	20.077	31.725	1.00	72.38

	975	СВ	LYS C	122	- 33.217	19.930	33.197	1.00	00.00
	976	CG	LYS C	122	33.582	21.162	34.003	1.00	98.98 98.98
	977	CD	LYS C	122	33.532	20.901	35.481	1.00	98.98
5	978 .	CE	LYS C	122	34.071	22.074	36.260	1.00	98.98
J	979 980	NZ C	LYS C LYS C	122 122	34.151 35.080	21.706 20.238	37.694	1.00	98.98
	981	ŏ	LYS C	122	35.836	19.379	31.595 32.017	1.00 1.00	72.38
	982	Ň	ASP C	123	35.507	21.342	31.001	1.00	72.38 92.01
10	983	CA	ASP C	123	36.918	21.628	30.809	1.00	92.01
10	984	CB	ASP C	123	37.606	21.819	32.161	1.00	107.76
	985 986	CG OD1	ASP C ASP C	123	37.288	23.167	32.785	1.00	107.76
	987	OD2	ASP C	123 123	37.362 36.979	24.186 23.215	32.052	1.00	107.76
	988	C	ASP C	123	37.613	20.553	34.000 29.996	1.00 1.00	107.76
15	889	Ō	ASP C	123	38.719	20.144	30.322	1.00	92.01 92.01
	990	N	GLY C	124	36.956	20.110	28.929	1.00	87.40
	991	CA	GLY C	124	37.516	19.094	28.054	1.00	87.40
	992 993	C O	GLY C GLY C	124 124	37.465	17.665	28.570	1.00	87.40
20	994	Ň	GLU C	125	37.795 37.047	16.741 17.474	27.826 29.821	1.00	87.40
	995	CA	GLU C	125	36.991	16.139	30.427	1.00 1.00	63.88 63.88
	996	CB	GLU C	125	37.331	16.197	31.931	1.00	184.13
	997	CG	GLU C	125	38.775	16.547	32.294	1.00	184.13
25	998	CD	GLU C	125	39.723	15.367	32.176	1.00	184.13
23	999 1000	OE1 OE2	GLU C	125 125	39.524	14.369	32.903	1.00	184.13
	1000	C	GLU C	125	40.665 35.626	15.445 15.490	31.359 30.284	1.00	184.13
	1002	ŏ	GLU C	125	34.611	16.164	30.370	1.00 1.00	63.88 63.88
••	1003	N	ALA C	126	35.587	14.182	30.067	1.00	91.37
30	1004	CA	ALA C	126	34.302	13.501	29.985	1.00	91.37
	1005	CB	ALA C	126	34.516	12.040	29.654	1.00	171.72
	1006 1007	C	ALA C ALA C	126 126	33.727 34.492	13.657	31.399	1.00	91.37
	1008	Ň	LEU C	127	32.410	13.626 13.835	32.369 31.533	1.00 1.00	91.37
35	1009	CA	LEU C	127	31.815	14.011	32.861	1.00	55.93 55.93
	1010	СВ	LEU C	127	31.291	15.421	33.033	1.00	79.78
	1011	CG	LEU C	127	31.277	15. 72 7	34.519	1.00	79.78
	1012 1013	CD1 CD2	LEU C	127	32.708	15.528	35.062	1.00	79.78
40	1014	C	LEU C	127 127	30.796 30.722	17.133 13.050	34.754 33.267	1.00 1.00	79.78
	1015	Ö	LEU C	127	30.851	12.396	34.292	1.00	55.93 55.93
	1016	N	LYS C	128	29.633	12.998	32.501	1.00	71.66
	1017	CA	LYS C	128	28.530	12.063	32.771	1.00	71.66
45	1018 1019	CB CG	LYS C Lys c	128 128	27.354	12,774	33.419	1.00	111.82
10	1020	CD	LYS C	128	27.672 27.814	13.421 12.412	34.740 35.853	1.00	111.82
	1021	CE	LYS C	128	27.997	13.133	37.204	1.00 1.00	111.82 111.82
	1022	NZ	LYS C	128	28.021	12.205	38.387	1.00	111.82
50	1023	C	LYS C	128	28.096	11.462	31.430	1.00	71.66
30	1024 1025	O N	LYS C Tyr C	128	28.281	12.090	30.386	1.00	71.66
	1026	CA	TYR C	129 129	27.537 27.110	10.252 9.616	31.447	1.00	51.68
	1027	CB	TYR C	129	28.197	8.680	30.208 29.692	1.00 1.00	51.68 75.51
	1028	CG	TYR C	129	27.655	7.647	28.732	1.00	75.51 75.51
55	1029	CD1	TYR C	129	27.412	7.957	27.399	1.00	75.51
	1030 1031	CE1	TYR C	129	26.846	7.041	26.529	1.00	75.51
	1032	CD2 CE2	TYR C TYR C	129 129	27.316 26.739	6.383	29.173	1.00	75.51
	1033	cz	TYR C	129	26.510	5.454 5.789	28.309 26.992	1.00 1.00	75.51
60	1034	ОН	TYR C	129	25.950	4.855	26.144	1.00	75.51 75.51
	1035	C	TYR C	129	25.817	8.822	30.371	1.00	51.68
	1036 1037	O _N	TYR C	129	25.656	8.097	31.360	1.00	51. 68
	1037	N CA	TRP C	130 130	24.912 23.641	8.945	29.390	1.00	122.00
65	1039	CB	TRP C	130	22.531	8.226 9.082	29.404 29.995	1.00	122.00
	1040	CG	TRP C	130	22.854	9.740	31.299	1.00 1.00	131.84 131.84
	1041	CD2	TRP C	130	22.370	9.360	32.590	1.00	131.84
	1042	CE2	TRP C	130	22.886	10.292	33.518	1.00	131.84
70	1043 1044	CE3 CD1	TRP C TRP C	130 130	21.557 23.613	8.317	33.053	1.00	131.84
. •		JD 1	mu. O	130	دا تا.ت	10.850	31.489	1.00	131.84

	1045 1046	NE1 CZ2	TRP C	130 130	23.636 22.613	11.194 10.216	32.819 34.887	1.00 1.00	131.84
	1047	CZ3	TRP C	130	21.283	8.239	34.422	1.00	131.84
	1048	CH2	TRP C	130	21.809	9.190	35.319	1.00	131.84 131.84
5	1049	C	TRP C	130	23.199	7.805	28.010	1.00	122.00
	1050	0	TRP C	130	23.720	8.292	27.015	1.00	122.00
	1051	N CA	TYR C	131	22.229	6.898	27.944	1.00	94.11
	1052 1053	CA CB	TYR C	131	21.710	6.443	26.663	1.00	94.11
10	1054	CG	TYR C	131 131	21.108 20.805	5.048 4.505	26.756	1.00	199.39
••	1055	CD1	TYR C	131	21.836	4.074	25.386 24.552	1.00 1.00	199.39
	1056	CE1	TYR C	131	21.583	3.681	23.247	1.00	199.39 199.39
	1057	CD2	TYR C	131	19.503	4.522	24.879	1.00	199.39
15	1058	CE2	TYR C	131	19.236	4.132	23.570	1.00	199.39
15	1059	CZ	TYR C	131	20.283	3.716	22.761	1.00	199.39
	1060 1061	C OH	TYR C	131	20.033	3.369	21.456	1.00	199.39
	1062	ŏ	TYR C	131 131	20.629 20.894	7.440 8.379	26.306	1.00	94.11
	1063	Ň	GLU C	132	19.411	7.221	25.554 26.817	1.00 1.00	94,11
20	1064	CA	GLU C	132	18.318	8.171	26.599	1.00	108.28 108.28
	1065	СВ	GLU C	132	16.986	7.670	27.185	1.00	249.42
	1066	CG	GLU C	132	16.250	6.597	26.375	1.00	249.42
	1067	CD	GLU C	132	14.874	7.058	25.901	1.00	249.42
25	1068 1069	OE1 OE2	GLU C	132	14.343	8.036	26.469	1.00	249.42
23	1070	C	GLU C	132 132	14.320 18.899	6.434 9.243	24.968	1.00	249.42
	1071	ŏ	GLU C	132	19.243	8.953	27.491 28.636	1.00 1.00	108.28
	1072	N	ASN C	133	19.029	10.468	26.989	1.00	108.28 132.29
	1073	CA	ASN C	133	19.665	11.502	27.790	1.00	132,29
30	1074	CB	ASN C	133	19.946	12.758	26.960	1.00	123.07
	1075	CG	ASN C	133	18.786	13.702	26.928	1.00	123.07
	1076 1077	OD1 ND2	ASN C ASN C	133	17.659	13.297	26.651	1.00	123.07
	1078	C	ASN C ASN C	133 133	19.047 18.983	14.979 11.879	27.200	1.00	123.07
35	1079	ŏ	ASN C	133	17.884	11.434	29.090 29.412	1.00 1.00	132.29 132.29
	1080	N	HIS C	134	19.677	12.730	29.824	1.00	77.87
	1081	CA	HIS C	134	19.271	13.173	31.140	1.00	77.87
	1082	CB	HIS C	134	20.089	12.388	32.162	1.00	247.23
40	1083 1084	CG CD2	HIS C	134	19.688	12.628	33.579	1.00	247.23
70	1085	ND1	HIS C	134 134	20.364 18.451	13.171	34.619	1.00	247.23
	1086	CE1	HIS C	134	18.385	12.270 12.581	34.071 35.352	1.00 1.00	247.23
	1087	NE2	HIS C	134	19.532	13.127	35.710	1.00	247.23 247.23
	1088	С	HIS C	134	19.573	14.664	31.255	1.00	77.87
45	1089	0	HIS C	134	19.843	15.338	30.252	1.00	77.87
	1090	N	ASN C	135	19.539	15.167	32.484	1.00	77.12
	1091 1092	CA CB	ASN C ASN C	135	19.779	16.576	32.747	1.00	77.12
	1093	CG	ASN C	135 135	18.442 17.690	17.308	32.868	1.00	227.67
50	1094	OD1	ASN C	135	18.287	17.335 17.624	31.558 30.520	1.00 1.00	227.67
	1095	ND2	ASN C	135	16.390	17.049	31.585	1.00	227.67 227.67
	1096	С	ASN C	135	20.595	16.748	34.004	1.00	77.12
	1097	0	ASN C	135	20.049	16.927	35.075	1.00	77.12
55	1098 1099	N CA	ILE C	136	21.914	16.671	33.862	1.00	56.71
55	1100	CA CB	ILE C	136	22.855	16.810	34.974	1.00	56.71
	1101	CG2	ILE C	136 136	24.267 24.215	17.147 18.298	34.439 33.4 6 8	1.00	111.08
	1102	CG1	ILE C	136	25.189	17.479	35.590	1.00 1.00	111.08 111.08
	1103	CD1	ILE C	136	26.605	17.684	35.143	1.00	111.08
60	1104	Ç	ILE C	136	22.387	17.870	35.956	1.00	56.71
	1105	0	ILE C	136	22.276	19.044	35.623	1.00	56.71
	1106	N OA	SER C	137	22.090	17.429	37.172	1.00	99.75
	1107 1108	CA CB	SER C SER C	137	21.594	18.308	38.225	1.00	99.75
65	1109	OG	SER C	137 137	20.218 19.833	17.820 18.438	38.673 39.884	1.00	125.93
	1110	č	SER C	137	22.517	18.411	39.884	1.00 1.00	125.93
	1111	Ö	SER C	137	23.195	17.457	39.807	1.00	99.75 99.75
	1112	N	ILE C	138	22.530	19.580	40.062	1.00	72.38
70	1113	CA	ILE C	138	23.366	19.816	41.235	1.00	72.38
70	1114	СВ	ILE C	138	24.560	20.663	40.881	1.00	52.39

	1115	CG2	ILE C	138	-25.241	21.106	42.161	1.00	52.39
	1116	CG1	ILE C	138	25.503	19.881	39.961	1.00	52.39
	1117	CD1	ILE C	138	26.574	20.747	39.311	1.00	52.39
5	1118 1119	C	ILE C	138	22.609	20.556	42.335	1.00	72.38
,	1120	N	THR C	138 139	22.109 22.535	21.667 19.955	42.112 43.51 9	1.00	72.38
	1121	CA	THR C	139	21.823	20.568	43.519 44.634	1.00 1,00	119.29
	1122	СВ	THR C	139	21.466	19.521	45.682	1.00	119.29 137.72
	1123	OG1	THR C	139	22.642	i 8.774	46.024	1.00	137.72
10	1124	CG2	THR C	139	20.404	18.578	45.139	1.00	137.72
	1125	C	THR C	139	22.679	21.655	45.275	1.00	119.29
	1126 1127	0 N	THR C ASN C	139 140	22.449	22.849	45.063	1.00	119.29
	1128	CA	ASN C	140	23.661 24.585	21.232 22.147	46.066 46.73€	1.00 1.00	83.41
15	1129	CB	ASN C	140	25.065	21.554	48.052	1.00	83.41 209.19
	1130	CG	ASN C	140	26.123	22.402	48.714	1.00	209.19
	1131	OD1	ASN C	140	27.087	22.824	48.073	1.00	209.19
	1132	ND2	ASN C	140	25.950	22.645	50.006	1.00	209.19
20	1133	C O	ASN C	140	25.758	22.277	45.780	1.00	83.41
20	1134 1135	N	ASN C ALA C	140 141	26.403 26.037	21.277	45.455	1.00	83.41
	1136	CA	ALA C	141	27.121	23.503 23.741	45.343 44.394	1.00 1.00	87.00
	1137	СВ	ALA C	141	26.704	24.753	43.381	1.00	-87. 00 58.59
	1138	С	ALA C	141	28.440	24.162	44.994	1.00	87.00
25	1139	0	ALA C	141	28.527	25 .112	45.753	1.00	87.00
	1140	N	THR C	142	29.485	23.450	44.617	1.00	69.33
	1141 1142	CA CB	THR C	142	30.822	23.733	45.106	1.00	69.33
	1143	OG1	THR C	142 142	31.688 31.001	22.461 21.383	45.035 45.687	1.00	195.23
30	1144	CG2	THR C	142	33.012	21.363 22.679	45.722	1.00 1.00	195.23 195.23
	1145	C	THR C	142	31.388	24.815	44.202	1.00	69.33
	1146	0	THR C	142	30.753	25.185	43.219	1.00	69.33
	1147	N	VAL C	143	32.561	25.341	44.531	1:00	71.38
35	1148	CA CB	VAL C	143	33.154	26.387	43.699	1.00	71.38
33	1149 1150	CG1	VAL C VAL C	143 143	34.082 35.270	27.349	44.511	1.00	62.36
	1151	CG2	VAL C	143	34.571	26.572 28.506	45.059 43.623	1.00 1.00	62.36 62.36
	1152	č	VAL C	143	33.989	25.686	42.654	1.00	71.38
40	1153	0	VAL C	143	34.383	26.277	41.655	1.00	71.38
40	1154	N	GLU C	144	34.272	24.416	42.897	1.00	78.73
	1155 1156	CA	GLU C	144	35.065	23,659	41.954	1.00	78.73
	1157	CB CG	GLU C	144 144	35.604 36.574	22.384 22.653	42.599	1.00	249.12
	1158	CD	GLU C	144	36.019	22.238	43.732 45.078	1.00 1.00	249.12
45	1159	OE1	GLU C	144	35.711	21.040	45.239	1.00	249.12 249.12
	1160	OE2	GLU C	144	35.889	23.102	45.972	1.00	249.12
	1161	Ç	GLU C	144	34.222	23.316	40.739	1.00	78.73
	1162	0	GLU C	144	34.767	22.933	39.711	1.00	78.73
50	1163 1164	N CA	ASP C ASP C	145 145	32.898	23.473	40.853	1.00	62,47
50	1165	CB	ASP C	145	31.977 30.545	23.174 23.066	39.754 40.260	1.00 1.00	62.47
•	1166	ČĠ	ASP C	145	30.305	21.798	41.028	1.00	127.97 127.97
	1167	OD1	ASP C	145	30.493	20.714	40.441	1.00	127.97
	1168	OD2	ASP C	145	29.935	21.883	42.217	1.00	127.97
55	1169	C	ASP C	145	32.053	24.220	38.663	1.00	62.47
	1170 1171	0 N	ASP C SER C	145	31.548	24.011	37.568	1.00	62.47
	1172	ČA	SER C	146 146	32.687 32.824	25.348 26.397	38.957	1.00	71.91
	1173	CB	SER C	146	33.438	27.641	37.960 38.599	1.00 1.00	71.91 151.98
60	1174	OG	SER C	146	32.599	28.127	39.630	1.00	151.98
	1175	Ç	SER C	146	33.711	25.866	36.837	1.00	71.91
	1176	O.	SER C	146	34.648	25.109	37.082	1.00	71.91
	1177 1178	N CA	GLY C GLY C	147	33.394	26.241	35.606	1.00	84.55
65	1179	CA	GLY C	147 147	34.170 33.449	25.785 26.062	34.466 33.158	1.00	84.55
	1180	ŏ	GLY C	147	32.552	26.062 26.898	33.158 33.121	1.00 1.00	84.55 84.55
	1181	Ň	THR C	148	33.836	25.373	32.084	1.00	54.14
	1182	CA	THR C	148	33.192	25.561	30.781	1.00	54.14
70	1183	CB	THR C	148	34.166	26.153	29.760	1.00	64.28
70	1184	OG1	THR C	148	34.588	25.133	28.858	1.00	64.28

	1185 1186	CG2 C	THR C	148 148	.35.394 32.671	26.717 24.216	30.474 30.285	1.00 1.00	64.28 54.14
	1187	0	THR C	148	33.429	23.287	30.032	1.00	54.14
_	1188	N	TYR C	149	31.359	24.119	30.145	1.00	33.05
5	1189	CA	TYR C	149	30.725	22.879	29.753	1.00	33.05
	1190	CB	TYR C	149	29.524	22.656	30.627	1.00	43.72
	1191	CG	TYR C	149	29.787	22.522	32.108	1.00	43.72
	1192	CD1	TYR C	149	30.185	23.612	32.391	1.00	43.72
10	1193 1194	CE1	TYR C	149	30.359	23.470	34.266	1.00	43.72
10	1195	CD2 CE2	TYR C	149	29.574	21.296	32.738	1.00	43.72
	1196	CZ	TYR C TYR C	149	29.739	21.143	34.095	1.00	43.72
	1197	OH	TYR C TYR C	149	30.130	22.222	34.876	1.00	43.72
	1198	C'	TYR C	149 149	30.255 30.257	22.023	36.258	1.00	43.72
15	1199	ŏ	TYR C	149	30.257	22.872 23.905	28.312	1.00	33.05
	1200	Ň	TYR C	150	29.929	21.687	27.666 27.818	1.00	33.05
	1201	CA	TYR C	150	29.402	21.473	26.481	1.00	75.60
	1202	СВ	TYR C	150	30.453	21.790	25.384	1.00 1.00	75.60
	1203	CG	TYR C	150	31.554	20.780	25.087	1.00	80.46
20	1204	CD1	TYR C	150	31.282	19.581	24.439	1.00	80.46
	1205	CT:	TYR C	150	32.288	18.664	24.162	1.00	80.46 80.46
	1206	CD2	TYR C	150	32.874	21.039	25.445	1.00	80.46
	1207	CE2	TYR C	150	33.889	20.130	25.168	1.00	80.46
25	1208	cz	TYR C	150	33.590	18.938	24.529	1.00	80.46
25	1209	ОН	TYR C	150	34.597	18.011	24.280	1.00	80.46
	1210	Ç	TYR C	150	28.963	20.007	26.498	1.00	75.60
	1211	0	TYR C	150	29.374	19.239	27.375	1.00	75.60
	1212	N	CYS C	151	28.090	19.604	25.586	1.00	100.28
30	1213	CA	CYS C	151	27.657	18.211	25.572	1.00	100.28
20	1214	C	CYS C	151	27.674	17.617	24.167	1.00	100.28
	1215 1216	O CB	CYS C	151	27.634	18.349	23.191	1.00	100.28
	1217	SG	CYS C	151	26.255	18.096	26.172	1.00	64.15
	1218	N N	CYS C THR C	151	24.959	19.135	25.424	1.00	64.15
35	1219	CA	THR C	152 152	27.746 27.755	16.291	24.074	1.00	69.97
	1220	CB	THR C	152	27.755 29.089	15.598	22.795	1.00	69.97
	1221	OG1	THR C	152	29.210	14.837 13.780	22.588 23.550	1.00	86.22
	1222	CG2	THR C	152	30.247	15.771	22.765	1.00 1.00	86.22
	1223	C	THR C	152	26.594	14.610	22.813	1.00	86.22 69.97
40	1224	0	THR C	152	26.242	14.082	23.879	1.00	69.97
	1225	N	GLY C	153	25.992	14.368	21.652	1.00	96.14
	1226	CA	GLY C	153	24.879	13,441	21.597	1.00	96.14
	1227	Ç	GLY C	153	24.588	13.010	20.182	1.00	96.14
45	1228	0	GLY C	153	25.037	13.663	19.247	1.00	96.14
45	1229	N	LYS C	154	23.845	11.918	20.017	1.00	77.66
	1230	CA	LYS C	154	23.522	11.431	18.690	1.00	77.66
	1231 1232	CB	LYS C	154	23.722	9.916	18.603	1.00	222.01
	1233	CD CD	LYS C	154	23.538	9.323	17.212	1.00	222.01
50	1234	CE	LYS C LYS C	154	23.820	7.833	17.253	1.00	222.01
50	1235	NZ	LYS C	154	23.556 23.726	7.151	15.924	1.00	222.01
	1236	Ċ	LYS C	154 154	23.726 22.086	5.689	16.075	1.00	222.01
	1237	ŏ	LYS C	154	21.221	11.796 11.567	18.428	1.00	77.66
	1238	Ň	VAL C	155	21.843	12.405	19.269	1.00	77.66
55	1239	CA	VAL C	155	20.496	12.796	17.271 16.862	1.00 1.00	110.66
	1240	CB	VAL C	155	20.397	14.288	16.585	1.00	110.66
	1241	CG1	VAL C	155	18.985	14.643	16.163	1.00	77.82 77.82
	1242	CG2	VAL C	155	20.778	15.046	17.834	1.00	77.82 77.82
	1243	С	VAL C	155	20.208	12.046	15.579	1.00	110.66
60	1244	0	VAL C	155	21.000	12.085	14.629	1.00	110.66
	1245	N	TRP C	156	19.074	11.363	15.553	1.00	192.10
	1246	CA	TRP C	156	18.727	10.560	14.401	1.00	192.10
	1247	CB	TRP C	156	18.811	11.362	13.120	1.00	246.44
65	1248	CG	TRP C	156	17.823	12.399	13.086	1.00	246.44
65	1249	CD2	TRP C	156	16.417	12.222	13.206	1.00	248.44
	1250	CE2	TRP C	156	15.830	13.503	13.150	1.00	246.44
	1251 1252	CE3	TRP C	156	15.592	11.100	13.355	1.00	246.44
	1252	CD1 NE1	TRP C	156	18.042	13.729	12.960	1.00	246.44
70	1254	CZ2	TRP C	156	16.846	14.407	13.005	1.00	246.44
. •		- Car	INF C	156	14.454	13.698	13.239	1.00	246.44

	1255	CZ3	TRP C	156	- 14.217	11.293	13.438	1.00	248.44
	1256	CH2	TRP C	156	13.662	12.588	13.378	1.00	246.44
	1257 1258	C	TRP C	156	19.771	9.496	14.335	1.00	192.10
5	1259	Ň	GLN C	156 157	19.673 20.800	8.478	15.006	1.00	192.10
•	1260	ČA	GLN C	157	21.861	9.769 8.814	13.545 13.373	1.00	118.64
	1261	CB	GLN C	157	21.511	7.931	12.180	1.00 1.00	118.64
	1262	CG	GLN C	157	20.361	6.995	12.528	1.00	249.64
	1263	CD	GLN C	157	20.670	6.255	13.803	1.00	249.64 249.64
10	1264	OE1	GLN C	157	21.748	5.725	13.918	1.00	249.64
	1265	NE2	GLN C	157	19.770	6.241	14.761	1.00	249.64
	1266	C	GLN C	157	23.230	9.430	13.234	1.00	118.64
	1267 1268	0 N	GLN C LEU C	157	24.183	8.768	12.826	1.00	118.64
15	1269	CA	LEU C	158 158	23.323 24.600	10.707	13.574	1.00	91.98
	1270	CB	LEU C	158	24.580	11.404 12.461	13.510	1.00	91.98
	1271	CG	LEU C	158	24.775	11.991	12.418 10.980	1.00 1.00	164.15
	1272	CD1	LEU C	158	25.736	12.973	10.359	1.00	164.15 164.15
	1273	CD2	LEU C	158	25.383	10.614	10.868	1.00	164.15
20	1274	Ç	LEU C	158	25.000	12.046	14.841	1.00	91.98
	1275	0	LEU C	158	24.147	12.397	15.658	1.00	91.98
	1276	N	ASP C	159	26.307	12.190	15.047	1.00	113.11
	1277 1278	CA CB	ASP C ASP C	159	26.839	12.762	16.273	1.00	113.11
25	1279	CG	ASP C	159 159	28.230 28.236	12.173	16.564	1.00	249.37
	1280	OD1	ASP C	159	27.536	10.645 10.057	16.599	1.00	249.37
	1281	OD2	ASP C	159	28.949	10.033	17.451 15.771	1.00	249.37
	1282	C	ASP C	159	26.939	14.280	16.148	1.00 1.00	249.37
	1283	0	ASP C	159	27.223	14.788	15.063	1.00	113.11 113.11
30	1284	N	TYR C	160	26.701	14.995	17.254	1.00	103.02
	1285	CA	TYR C	160	26.782	16.464	17.278	1.00	103.02
	1286	CB	TYR C	160	25.424	17.105	17.057	1.00	177.48
	1287	CG	TYR C	160	24.711	16.622	15.826	1.00	177.48
35	1288 1289	CD1 CE1	TYR C TYR C	160	23.860	15.521	15.882	1.00	177.48
55	1290	CD2	TYR C	160 160	23.204 24.891	15.062 17.255	14.752	1.00	177.48
	1291	CE2	TYR C	160	24.241	18.804	14.600 13.458	1.00 1.00	177.48
	1292	CZ	TYR C	160	23.400	15.707	13.545	1.00	177.48 177.48
	1293	OH	TYR C	160	22.763	15.245	12.427	1.00	177.48
40	1294	Ç	TYR C	160	27.333	16.998	18.581	1.00	103.02
	1295	0	TYR C	160	27.095	16.449	19.647	1.00	103.02
	1296 1297	N	GLU C	161	28.052	18.102	18.474	1.00	74.72
	1297	CA CB	GLU C	161	28.687	18.775	19.599	1.00	74.72
45	1299	CG	GLU C	161	30.170	18.972	19.273	1.00	249.14
	1300	CD	GLU C	161 161	30.978 32.456	19. 72 9 19.531	20.300	1.00	249.14
	1301	OE1	GLU C	161	33.259	20.350	20.085 20.582	1.00 1.00	249.14
	1302	OE2	GLU C	161	32.808	18.538	19,417	1.00	249.14 249.14
~~	1303	С	GLU C	161	27.985	20.117	19.779	1.00	74.72
50	1304	0	GLU C	161	27.656	20.780	18.806	1.00	74.72
	1305	N	SER C	162	27.743	20.516	21.021	1.00	59.53
	1306 1307	CA	SER C	162	27.055	21.776	21.320	1.00	59.53
	1307	CB OG	SER C	162	26.210	21.627	22.573	1.00	71.52
55	1309	C	SER C SER C	162 162	27.017 28.038	21.253	23.673	1.00	71.52
	1310	ŏ	SER C	162	29.247	22.914 22.679	21.532	1.00	59.53
	1311	Ň	GLU C	163	27.521	24.145	21. 60 8 21. 6 15	1.00 1.00	59.53
	1312	CA	GLU C	163	28.371	25.330	21.810	1.00	68.20 68.20
<i>~</i>	1313	CB	GLU C	163	27.580	26.610	21.565	1.00	172.64
60	1314	CG	GLU C	163	27.289	26.902	20.098	1.00	172.64
	1315	CD	GLU C	163	28.513	27.375	19.334	1.00	172.64
	1316	OE1	GLU C	163	29.120	28.383	19.757	1.00	172.64
	1317 1318	OE2	GLU C	163	28.864	26.748	18.311	1.00	172.64
65	1319	C	GLU C	163 163	28.856	25.296	23.246	1.00	68.20
	1320	Ň	PRO C	164	28.104 30.123	24.920 25.682	24.131	1.00	68.20
	1321	CD	PRO C	164	31.163	25.683 26.188	23.498 22.601	1.00	54.78
	1322	CA	PRO C	164	30.609	25.645	24.876	1.00 1.00	96.83 54.78
70	1323	CB	PRO C	164	32.109	25.851	24.709	1.00	96.83
70	1324	CG	PRO C	164	32.176	26.765	23.584	1.00	96.83

	1325	C	PRO C	164	- 29.950	26.720	25.688	1.00	54.78
	1326 1327	. O	PRO C	164	29.480	27.695	25.137	1.00	54.78
	1328	CA	LEU C	165 165	29.898 29.272	26.537 27.513	27.000 27.861	1.00	73.43
5	1329	CB	LEU C	165	27.829	27.112	28.127	1.00 1.00	73.43 54.02
	1330	CG	LEU C	165	27.163	27.955	29.201	1.00	54.02
	1331	CD1	LEU C	165	27.395	29.384	28.820	1.00	54.02
	1332 1333	CD2	LEU C	165	25.690	27.665	29.329	1.00	54.02
10	1334	C	LEU C	165 165	30.010 30.200	27.634 26.641	29.164	1.00	73.43
	1335	Ň	ASN C	166	30.420	28.853	29.859 29.493	1.00 1.00	73.43
	1336	CA	ASN C	166	31.148	29.098	30.736	1.00	53.84 53.84
	1337	CB	ASN C	166	31.979	30.368	30.646	1.00	80.99
15	1338	CG	ASN C	166	33.392	30.110	30.181	1.00	80.99
13	1339 1340	OD1 ND2	ASN C	166	33.956	29.054	30.431	1.00	80.99
	1341	C	ASN C	166 166	33.973 30.233	31.096 29.236	29.516 31.918	1.00 1.00	80.99
	1342	ŏ	ASN C	166	29.145	29.756	31.789	1.00	53.84 53.84
	1343	N	ILE C	167	30.693	28.806	33.084	1.00	65.33
20	1344	CA	ILE C	167	29.878	28.881	34.292	1.00	65.33
	1345	CB	ILE C	167	29.218	27.527	34.603	1.00	38.60
	1346 1347	CG2 CG1	ILE C	167	28.736	27.503	36.027	1.00	38.60
	1348	CD1	ILE C	167 167	28.066 27.261	27.269 26.070	33.618	1.00	38.60
25	1349	C.	ILE C	167	30.717	29.258	33.933 35.475	1.00 1.00	38.60
	1350	Ō	ILE C	167	31.781	28.681	35.694	1.00	65.33 65.33
	1351	N	THR C	168	30,110	30.223	36.246	1.00	
	1352	CA	THR C	168	31.015	30.619	37.406	1.00	58.90
30	1353	CB	THR C	168	31.537	32.023	37.260	1.00	100.28
30	1354 1355	OG1 CG2	THR C	168	32.315	32.110	36.067	1.00	100.28
	1356	C	THR C	168 168	32.406 30.230	32.354 30.502	38.4 3 8 38.708	1.00 1.00	100.28
	1357	ŏ	THR C	168	29.042	30.852	38.795	1.00	58.90 58.90
	1358	N	VAL C	169	30.908	29.965	39.708	1.00	74.23
35	1359	CA	VAL C	169	30.337	29.795	41.021	1.00	74.23
	1360	CB	VAL C	169	30.424	28.330	41.467	1.00	86.72
	1361 1362	CG1 CG2	VAL C	169	30.314	28.229	42.962	1.00	86.72
	1363	C	VAL C	169 169	29. 323 31.196	27.547 30.668	40.813 41.924	1.00 1.00	86.72
40	1364	ŏ	VAL C	169	32.359	30.328	42.184	1.00	74.23 74.23
	1365	N	ILE C	170	30.645	31.805	42.365	1.00	66.08
	1366	CA	ILE C	170	31.376	32.711	43.252	1.00	66.08
	1367 1368	CB	ILE C	170	30.995	34.166	42.997	1.00	82.85
45	1369	CG2 CG1	ILE C	170 170	31.079	34.476	41.520	1.00	82.85
1.5	1370	CD1	ILE C	170	29.572 29.097	34.412 35.848	43.431 43.156	1.00 1.00	82.85
	1371	Č.	ILL C	170	31.092	32.355	44.701	1.00	82.85 66.08
	1372	0	ILE C	170	30.272	31.482	44.960	1.00	66.08
50	1373	N.	LYS C	171	31.771	32.999	45.644	1.00	110.58
30	1374 1375	CA CB	LYS C	171	31.545	32.688	47.052	1.00	110.58
	1376	CG	LYS C	171 171	32.749 34.062	31.935	47.625	1.00	192.81
	1377	CD	LYS C	171	35.247	32.679 31.723	47.478 47.505	1.00	192.81
	1378	CE	LYS C	171	35.319	30,934	47.505 48.803	1.00 1.00	102.81 192.81
55	1379	NZ	LYS C	171	36.464	29.978	48.796	1.00	192.81
	1380	C	LYS C	171	31.263	33.931	47.882	1.00	110.58
	1381 1382	0	LY3 C	171	30.884	33.830	49.050	1.00	110.58
	1383	C1 C2	NAG C	221 221	4.609	28.125	21.539	1.00	248.09
60	1384	N2	NAG C	221	4.738 6.129	26.611 26.254	21.473 21.269	1.00 1.00	248.09 248.09
	1385	C7	NAG C	221	6.578	25.075	21.680	1.00	248.09
	1386	07	NAG C	221	5.867	24.254	22.257	1.00	248.09
	1387	C8	NAG C	221	8.042	24.762	21.420	1.00	248.09
65	1388	C3	NAG C	221	3.908	26.047	20.327	1.00	248.09
0 5	1389 1390	03 C4	NAG C	221 221	3.902	24.630	20.401	1.00	248.09
	1391	04 04	NAG C	221 221	2.465 1.852	26.559 26.163	20.341 19.095	1.00	248.09
	1392	C5	NAG C	221	2.447	28.096	20.488	1.00 1.00	248.09 248.09
-	1393	O 5	NAG C	221	3.226	28.499	21.641	1.00	248.09
70	1394	C6	NAG C	221	1.052	28.659	20.692	1.00	248.09

	1395	O 6	NAG C	221	- 0.460	28.142	21.875	1.00	248.09
	1396	C1	NAG C	222	0.468	26.179	18.986	1.00	248.99
	1397 1398	C2	NAG C	222	-0.014	24.897	18.283	1.00	248.99
5	1399	N2 C7	NAG C	222 222	0.382 -0.541	23.729	19.048	1.00	248.99
3	1400	07	NAG C	222	-0.541 -1.750	22.909 23.088	19.543 19.392	1.00	248.99
	1401	C8	NAG C	222	-0.046	21.704	20.330	1.00 1.00	248.99
	1402	C3	NAG C	222	0.566	24.815	16.861	1.00	248.99 248.99
	1403	O 3	NAG C	222	-0.012	23.714	16.171	1.00	248.99
10	1404	C4	NAG C	222	0.292	26.112	16.083	1.00	248.99
	1405	04 05	NAG C	222	0.989	26.082	14.843	1.00	248.99
	1406 1407	C5 O5	NAG C NAG C	222	0.742	27.337	16.897	1.00	248.99
	1408	C6	NAG C	222 222	0.107 0.396	27.330 28.661	18.201 16.232	1.00	248.99
15	1409	06	NAG C	222	1.499	29.556	16.260	1.00 1.00	248.99
	1410	C1	NAG C	242	18.858	43.706	21.097	1.00	248.99 98.91
	1411	C2	NAG C	242	18.159	43.460	19.760	1.00	98.91
	1412	N2	NAG C	242	16.728	43.568	19.914	1.00	98.91
20	1413 1414	C7	NAG C	242	16.062	44.435	19.166	1.00	98.91
20	1415	O7 C8	NAG C NAG C	242 242	16.610	45.163	18.336	1.00	98.91
	1416	čš	NAG C	242	14.561 18.507	44.512 42.075	19.366 19.237	1.00 1.00	98.91
	1417	03	NAG C	242	17.925	41.880	17.955	1.00	98.91 98.91
	1418	C4	NAG C	242	20.020	41.925	19.144	1.00	98.91
25	1419	04	NAG C	242	20.340	40.556	18.833	1.00	98.91
	1420	C5	NAG C	242	20.708	42.318	20.459	1.00	98.91
	1421	O5	NAG C	242	20.270	43.615	20.916	1.00	98.91
	1422 1423	C6 O6	NAG C NAG C	242	22.196	42.434	20.243	1.00	98.91
30	1424	C1	NAG C	242 243	22.917 20.966	41.643 40.334	21.170 17.621	1.00 1.00	98.91
	1425	C2	NAG C	243	21.805	39.050	17.674	1.00	148.54 148.54
	1426	N2	NAG C	243	22.863	39.159	18.662	1.00	148.54
	1427	C7	NAG C	243	23.081	38.154	19.504	1.00	148.54
35	1428	07	NAG C	243	22.402	37.126	19.506	1.00	148.54
33	1429 1430	C8 . C3	NAG C	243	24.212	38.320	20.503	1.00	148.54
	1431	03	NAG C NAG C	243 243	22.422 23.126	38.803 37.573	16.299 16.300	1.00	148.54
	1432	č4	NAG C	243	21.341	38.791	15.201	1.00 1.00	148.54 148.54
	1433	04	NAG C	243	21.974	38.713	13.890	1.00	148.54
40	1434	C5	NAG C	243	20.529	40.090	15.296	1.00	148.54
	1435	O5	NAG C	243	19.954	40.216	16.611	1.00	148.54
	1436 1437	C6	NAG C	243	19.402	40.197	14.299	1.00	148.54
	1438	O6 C1	NAG C MAN C	243 244	18.380 21.585	39.264	14.597	1.00	148.54
45	1439	Č2	MAN C	244	21.654	37.818 36.312	12.938 13.272	1.00 1.00	182.20 182.20
	1440	02	MAN C	244	20.383	35.858	13.660	1.00	182.20
	1441	C3	MAN C	244	22.042	35.694	11.892	1.00	182.20
	1442	03	MAN C	244	22.157	34.284	11.945	1.00	182.20
50	1443	C4	MAN C	244	21.095	36.131	10.730	1.00	182.20
50	1444 1445	O4 C5	MAN C MAN C	244 244	^1.496	35.520	9.503	1.00	182.20
	1446	O5	MAN C	244	≥1.199 20.771	37.666 38.312	10.607 11.834	1.00 1.00	182.20
	1447	Č6	MAN C	244	20.464	38.264	9.406	1.00	182.20 182.20
	1448	O6	MAN C	244	19.092	38.434	9.670	1.00	182.20
55	1449	C1	NAG C	250	-1.001	38.689	31.557	1.00	249.77
	1450	C2	NAG C	250	-1.761	27.609	32.354	1.00	249.77
	1451 1452	N2 C7	NAG C	250	-1.602	37.821	33.782	1.00	249.77
	1453	07	NAG C NAG C	250 250	-2.636 -2.781	38.209	34.526	1.00	249.77
60	1454	C8	NAG C	250 250	-3.761 -2.384	38.414 38.404	34.060 36.016	1.00 1.00	249.77
	1455	œ	NAG C	250	-1.221	36.224	31.975	1.00	249.77 249.77
	1456	03	NAG C	250	-1.975	35.209	32.626	1.00	249.77
	1457	C4	NAG C	250	-1.287	36.028	30.458	1.00	249.77
65	1458	04 05	NAG C	250	-0.662	34.799	30.113	1.00	249.77
O)	1459 1460	C5 O5	NAG C NAG C	250 250	-0.582	37.194	29.736	1.00	249.77
	1461	C6	NAG C	250 250	-1.150 -0.717	38.457 37.121	30.150 28.224	1.00	249.77
	1462	06	NAG C	250	-0.717 -0.351	37.121 38.351	28.224 27.612	1.00 1.00	249.77 249.77
-	1463	C1	NAG C	274	16.034	53.837	43.921	1.00	249.77 248.46
70	1464	C2	NAG C	274	17.088	53.346	44.921	1.00	248.46

	1465	N2	NAG C	274	. 16.465	52.511	45.928	1.00	248.46
	1466 1467	C7 O7	NAG C	274	17.189	51.604	46.575	1.00	248.46
٧.	1467	C8	NAG C NAG C	274 274	18.387	51.422	46.354	1.00	248.46
5	1469	Č	NAG C	274	16.474 17.768	50.767 54.539	47.625 45.598	1.00	248.46
-	1470	03	NAG C	274	18.835	54.081	45.586 46.416	1.00 1.00	248.46
	1471	C4	NAG C	274	18.306	55.518	44.553	1.00	248.46 248.46
•	1472	04	NAG C	274	18.793	56.685	45.202	1.00	248.46
10	1473	C5	NAG C	274	17.195	55.898	43.563	1.00	248.46
10	1474	O5	NAG C	274	16.641	54.710	42.959	1.00	248.46
	1475 1476	C6 O6	NAG C NAG C	274	17.688	56.784	42.432	1.00	248.46
	1477	C1	NAG C	274 335	16.703 15.450	56.920 18.012	41.418 31.039	1.00	248.46
	1478	C2	NAG C	335	14.351	18.418	C2.049	1.00 1.00	249.77
15	1479	N2	NAG C	335	14.844	18.144	3.1.387	1.00	249.77 249.77
	1480	C 7	NAG C	335	15.027	19.131	£4.258	1.00	249.77
	1481	07	NAG C	3 35	14.782	20.312	31.004	1.00	249.77
	1482 1483	C8 C3	NAG C	335	15.555	18.743	35.627	1.00	249.77
20	1484	O3	NAG C NAG C	335 335	13.010 11.981	17.686	31.860	1.00	249.77
	1485	C4	NAG C	335	12.654	18.411 17.546	32.519 30.386	1.00 1.00	249.77
	1486	04	NAG C	335	11.455	16.796	30.245	1.00	249.77 249.77
	1487	C5	NAG C	335	13.801	16.839	29.679	1.00	249.77 249.77
25	1488	O5	NAG C	335	14.974	17.683	29.710	1.00	249.77
25	1489	C6	NAG C	335	13.481	16.566	28.214	1.00	249.77
	1490 1491	O6 C1	NAG C	335	13.512	15.176	27.922	1.00	249.77
	1492	C2	NAG C NAG C	340 340	26.860 27.612	22.059 23.165	50.969	1.00	249.77
	1493	N2	NAG C	340	28.257	24.040	51.681 50.724	1.00 1.00	249.77
30	1494	C7	NAG C	340	28.068	25.353	50.821	1.00	243.77 249.77
	1495	07	NAG C	340	27.368	25.865	51.703	1.00	249.77
	1496	C8	NAG C	340	28.755	26.232	49.794	1.00	249.77
	1497 1498	C3 O3	NAG C	340	28.630	22.560	52.634	1.00	249.77
35	1499	03 C4	NAG C NAG C	340 340	29.275 27.915	23.608 21.620	53.354	1.00	249.77
	1500	04	NAG C	340	28.896	20.922	53.612 54. 36 5	1.00 1.00	249.77 249.77
	1501	C5	NAG C	340	26.987	20.611	52.880	1.00	249.77
	1502	O 5	NAG C	340	26.141	21.281	51.923	1.00	249.77
40	1503	C6	NAG C	340	26.045	19.869	53.817	1.00	249.77
40	1504 1505	O6 C1	NAG C NAG C	340	24.805	19.571	53.193	1.00	249.77
	1506	C2	NAG C	366 366	35.293 35.391	30.923 31.732	28.965	1.00	158.36
	1507	N2	NAG C	366	34.394	31.261	27.687 26.748	1.00 1.00	158.36
	1508	C7	NAG C	366	33,197	31.835	26.713	1.00	158.36 158.36
45	1509	07	NAG C	366	32.885	32.778	27.446	1.00	158.36
	1510	C8	NAG C	366	32.191	31.285	25.707	1.00	158.36
	1511 1512	C3 O3	NAG C NAG C	366	36.780	31.584	27.089	1.00	158.36
	1513	Ω Ω	NAG C	366 366	36.910 37.866	32.461	25.981	1.00	158.36
50	1514	04	NAG C	366	39.144	31.903 31.523	28.119 27.5 7 3	1.00 1.00	158.36 158.36
	1515	C5	NAG C	366	37.620	31.138	29.429	1.00	158.36
	1516	O 5	NAG C	366	36.277	31.367	29.896	1.00	158.36
	1517	C6	NAG C	366	38.550	31.570	30.549	1.00	158.36
55	1518` 1519	O6	NAG C	366	38.325	30.807	31.727	1.00	158.36
<i>J J</i>	1520	C1 C2	NAG C NAG C	367 367	40.136	32.494	27.559	1.00	249.59
	1521	N2	NAG C	367	41.511 41.702	31.828 30.834	27.487 28.613	1.00 1.00	249.59
	1522	C7	NAG C	367	41.695	29.619	28.418	1.00	249.59 249.59
4 0	1523	07	NAG C	367	41.532	29.106	27.308	1.00	249.59
60	1524	C8	NAG C	367	41.899	28.735	29.639	1.00	249.59
	1525 1526	C3 O3	NAG C	367	42.590	32.914	27.465	1.00	249.59
	1527	64 64	NAG C NAG C	367 367	43.877 42.343	32.321 33.850	27.352	1.00	249.59
	1528	04	NAG C	367 367	42.343 43.281	33.850 34.917	26.278 26.303	1.00	249.59
65	1529	C5	NAG C	367	40.913	34.411	26.335	1.00 1.00	249.59 249.59
	1530	O5	NAG C	367	39.945	33.331	26.405	1.00	249.59 249.59
	1531	C6	NAG C	367	40.576	35.245	25.112	1.00	249.59
	1532 1533	O6 CB	NAG C	367	39.610	34.604	24.292	1.00	249.59
70	1534	CG	LYS A LYS A	4	5.822	17.052	16.197	1.00	225.85
. •			LIG A	7	4.918	18.220	15.853	1.00	225.85

	1535	CD	LYS A	4	4.535	18.995	17.100	1.00	225.85
	1536 1537	CE	LYS A	4	3.638	20.173	16.766	1.00	225.85
	1537	NZ C	LYS A	4	3.267	20.934	17.987	1.00	225.85
5	1539	ŏ	LYS A	4	7.001 7.491	17. 23 9 18. 2 92	14.016	1.00	249.21
_	1540	Ň	LYS A	4	7.236	15.183	14.419 15.408	1.00	249.21
	1541	CA	LYS A	4	6.316	16.275	14.978	1.00 1.00	249.21
	1542	N	PRO A	5	7.053	- 16.880	12.723	1.00	249.21 94.49
10	1543	CD	PRO A	5	6.773	15.535	12.187	1.00	84.99
10	1544	CA	PRO A	5	7.685	17.735	11.709	1.00	94.49
	1545	CB	PRO A	5	8.092	16.736	10.629	1.00	84.99
	1546 1547	CG C	PRO A	5	7.010	15.716	10.691	1.00	84.99
	1548	ŏ	PRO A PRO A	5 5	6.772	18.825	11.164	1.00	94.49
15	1549	Ň	LYS A	6	5.557 7.358	18.721 19.877	11.227	1.00	94.49
	1550	CA	LYS A	6	6.559	20.973	10.617 10.084	1.00	99.70
	155 i	СВ	LYS A	6	6.444	22.094	11.130	1.00 1.00	99.70
	1552	CG	LYS A	6	5.540	23.242	10.711	1.00	128.86 128.86
20	1553	CD	LYS A	6	5.290	24.223	11.853	1.00	128.86
20	1554	CE	LYS A	6	4.321	25.32 9	11.418	1.00	128.86
	1555	NZ	LYS A	6	3.977	26.285	12.517	1.00	128.86
	1556 1557	CO	LYS A	6	7.166	21.512	8.793	1.00	99.70
	1558	N	LYS A VAL A	6	8.281	22.029	8.801	1.00	99.70
25	. 1559	ČA	VAL A	7 7	6.421	21.395	7.693	1.00	71.19
	1560	CB	VAL A	7	6.878 5.955	21.852 21.392	6.377	1.00	71.19
	1561	CG1	VAL A	7	6.584	21.739	5.243 3. 9 00	1.00 1.00	54.73
	1562	CG2	VAL A	7	5.687	19.922	5.350	1.00	54.73
20	1563	С	VAL A	7	6.947	23.354	6.221	1.00	54.73 71.19
30	1564	0	VAL A	7	5.924	24.023	6.282	1.00	71.19
	1565	N	SER A	8	8.141	23.885	5.988	1.00	76.52
	1566 1567	CA	SER A	8	8.301	25.325	5.804	1.00	76.52
	1568	CB OG	SER A	8	9.537	25.827	6.563	1.00	232.80
35	1569	Č	SER A SER A	8 8	10.701 8.437	25.106	6.196	1.00	232.80
	1570	ŏ	SER A	8	8.665	25.597 24.679	4.311 3.534	1.00	76.52
	1571	N	LEU A	9	8.274	26.851	3.914	1.00 1.00	76.52
	1572	CA	LEU A	9	8.388	27.237	2.509	1.00	77.48 77.48
40	1573	CB	LEU A	9	7.037	27.651	1.935	1.00	70.08
40	1574	CG	LEU A	9	5.879	26.663	1.868	1.00	70.08
	1575 1576	CD1	LEU A	9	4.901	27.105	0.816	1.00	70.08
	1577	CD2 C	LEU A LEU A	9	6.399	25.305	1.517	1.00	70.08
	1578	ŏ	LEU A	9 9	9.321	28.417	2.334	1.00	77.48
45	1579	Ň	ASN A	10	9.506 9.896	29.212 28.544	3.257	1.00	77.48
	1580	CA	ASN A	10	10.795	29.657	1.140 0.844	1.00 1.00	96.41
	1581	CB	ASN A	10	12.196	29.384	1.384	1.00	96.41 121.54
	1582	CG	ASN A	10	13.074	30.616	1.338	1.00	121.54
50	1583	OD1	ASN A	10	12.819	31.598	2.041	1.00	121.54
50	1584 1585	ND2	ASN A	10	14.108	30.581	0.496	1.00	121.54
	1586	C	ASN A	10	10.868	29.920	-0.654	1.00	96.41
	1587	Ň	ASN A PRO A	10	11.396	29.110	-1.412	1.00	96.41
	1588	CD	PRO A	11 11	10.325 10.263	31.064 31.320	-1.105	1.00	78.36
55	1589	CA	PRO A	11	9.642	32.128	-2.548 -0.350	1.00	72.21
	1590	CB	PRO A	11	9.130	33.049	-0.330 -1.455	1.00 ·· 1.00	78.36
	1591	CG	PRO A	11	10.084	32.803	-2.583	1.00	72.21 72.21
	1592	C	PRO A	11	8.492	31.647	0.551	1.00	78.36
60	1593	0	PRO A	11	7.992	30.537	0.386	1.00	78.36
00	1594 1595	N CD	PRO A	12	8.056	32.469	1.513	1.00	81.66
	1596	GA	PRO A PRO A	12	8.570	33.812	1.833	1.00	122.93
	1597	CB	PRO A	12 12	6.968 6.925	32.110	2.430	1.00	81.66
	1598	ČĞ	PRO A	12	8.277	33.274 33.895	3.409	1.00	122.93
65	1599	C	PRO A	12	5.637	31.998	3.290 1.663	1.00 1.00	122.93
	1600	0	PRO A	12	4.695	31.307	2.081	1.00	81.66 81.66
	1601	N _.	TRP A	13	5.579	32.699	0.538	1.00	66.49
	1602	CA	TRP A	13	4.388	32.725	-0.293	1.00	66.49
70	1603 1604	CB CC	TRP A	13	4.660	33.539	-1.562	1.00	100.34
,,	1004	CG	TRP A	13	5.336	34.831	-1.277	1.00	100.34

	1605 1606	CD2 CE2	TRP A	13 13	- 5.100 6.000	35.697 36.762	-0.167 -0.268	1.00 1.00	100.34 100.34
	1607	CE3	TRP A	13	4.210	35.673	0.909	1.00	100.34
_	1608	CD1	TRP A	13	6.339	35.393	-1.996	1.00	100.34
5	1609	NET	TRP A	13	6.748	36.552	-1.395	1.00	100.34
	1610	CZ2	TRP A	13	6.046	37.795	0.664	1.00	100.34
	1611	CZ3	TRP A	13	4.253	36.698	1.829	1.00	100.34
	1612	CH2	TRP A	13	5.167	37.745	1.705	1.00	100.34
10	1613	C	TRP A	13 -	3.913	31.342	-0.666	1.00	66.49
10	1614 1615	0 N	TRP A	13	4.637	30.573	-1.270	1.00	66.49
	1616	CA	ASN A ASN A	14 14	2.685 2.109	31.031	-0.299	1.00	52.07
	1617	CB	ASN A	14	1.508	29.738 29.082	-0. 62 9 0. 62 6	1.00	52.07
	1618	ČĞ	ASN A	14	0.274	29.801	1.152	1.00 1.00	104.36
15	1619	OD1	ASN A	14	0.305	31.001	1.465	1.00	104.36 104.36
	1620	ND2	ASN A	14	-0.822	29.058	1.269	1.00	104.36
	1621	С	ASN A	14	1.056	29.792	-1.759	1.00	52.07
	1622	0	ASN A	14	0.271	28.850	-1.928	1.00	52.07
20	1623	N	ARG A	15	1.026	30.900	-2.509	1.00	52.98
20	1624	CA	ARG A	15	0.131	31.078	-3.667	1.00	52.98
	1625	CB	ARG A	15	-0.942	32.109	-3.415	1.00	66.97
	1626	CG	ARG A	15	-1.533	32.043	-2.077	1.00	66.97
	1627 1628	CD NE	ARG A	15	-2.626	33.064	-2.014	1.00	66.97
25	1629	CZ	ARG A ARG A	15 15	-3.768	32.699	-2.837	1.00	66.97
	1630	NH1	ARG A	15	-4.589 -4.370	33.596 34.890	-3.363	1.00	66.97
	1631	NH2	ARG A	15	-5.6 29	33.213	-3.150 -4.091	1.00 1.00	66.97
	1632	C	ARG A	15	1.080	31.659	-4.687	1.00	66.97 52.98
	1633	Õ	ARG A	15	1.510	32.817	-4.563	1.00	52.98
30	1634	N	ILE A	16	1.431	30.867	-5.684	1.00	61.11
	1635	CA	ILE A	16	2.362	31.362	-6.667	1.00	61.11
	1636	CB	ILE A	16	3.662	30.595	-6.632	1.00	64.67
	1637	CG2	ILE A	16	4.375	30.856	-5.312	1.00	64.67
35	1638	CG1	ILE A	16	3.385	29.117	-6.833	1.00	64.67
33	1639 1640	CD1 C	ILE A	16	4.626	28.268	-6.768	1.00	64.67
	1641	ŏ	ILE A	16 16	1.849 0.851	31.311	-8.070	1.00	61.11
	1842	Ň	PHE A	17	2.560	30.662 32.019	-8.361 -8.933	1.00 1.00	61.11
	1643	ČA	PHE A	17	2.266	32.130	-0.933 -10.348	1.00	81.85 81.85
40	1644	CB	PHE A	17	2.902	33.411	-10.856	1.00	58.17
	1645	CG	PHE A	17	2.014	34.604	-10.777	1.00	58.17
	1646	CD1	PHE A	17	2.531	35.841	-10.422	1.00	58.17
	1647	CD2	PHE A	17	0.681	34.512	-11.181	1.00	58.17
45	1648	CE1	PHE A	17	1.751	36.96 5	-10.467	1.00	58.17
45	1649	CE2	PHE A	17	-0.125	35.639	-11.238	1.00	58.17
	1650	CZ	PHE A	17	0.415	36.876	-10.885	1.00	58.17
	1651 1652	C	PHE A PHE A	17	2.851 3.749	30.940	-11.110	1.00	81.85
	1653	Ň	LYS A	17 18	3.749 2.353	30.259	-10.621	1.00	81.85
50	1654	ČA	LYS A	18	2.842	30.699 29.602	-12.314 -13.129	1.00	81.40
	1655	CB	LYS A	18	1.981	29.497	-13.129 -14.385	1.00 1.00	81.40
	1656	ĊĠ	LYS A	18	2.281	28.313	-15.277	1.00	133.55 133.55
	1657	CD	LYS A	18	1.153	28.136	-16.287	1.00	133.55
	1658	CE	LYS A	18	1.389	26.957	-17.216	1.00	133.55
55	1659	NZ .	LYS A	18	2.627	27.139	-18.030	1.00	133.55
	1660	Č	LYS A	18	4.305	29.838	-13.515	1.00	81,40
	1661	0	LYS A	18	4.683	30.921	-13.972	1.00	81.40
	1662	N	GLY A	19	5.141	28.834	-13.313	1.00	92.32
60	1663 1664	CA	GLY A	19	6.524	28.975	-13.702	1.00	92.32
00	1665	C	GLY A GLY A	19	7.492	29.428	-12.643	1.00	92.32
	1666	Ň	GLU A	19 20	8.697 6.996	29.398 29.853	-12.866 -11.401	1.00	92.32
	1667	ČA	GLU A	20	7.896	29.653 30.300	-11.491 -10.422	1.00 1.00	67.13 67.13
	1668	CB	GLU A	20	7.153	31.239	-10.422 -9.477	1.00	67.13 115.51
65	1669	CG	GLU A	20	6.439	32.361	-10.221	1.00	115.51
	1670	CD	GLU A	20	5.794	33.361	-9.300	1.00	115.51
	1671	OE1	GLU A	20	4.991	32.949	-8.432	1.00	115.51
	1672	OE2	GLU A	20	6.091	34.561	-9.454	1.00	115.51
70	1673	C	GLU A	20	8.469	29.094	-9.652	1.00	67.13
70	1674	0	GLU A	20	8.035	27.953	-9.861	1.00	67.13

	4075	N	4001 4	•					,
	1675	N CA	ASN A	21	9.456	29.329	-8.788	1.00	81.05
	1676	CA	ASN A	21	10.059	28.225	-8.040	1.00	81.05
	1677	CB	ASN A	21	11.562	28.078	-8.328	1.00	110.52
5	1678	CG	ASN A	21	11.923	28.283	-9.788	1.00	110.52
3	1679	OD1	ASN A	21	11.250	27.808	-10.699	1.00	110.52
	1680	ND2	ASN A	21	13.025	28.989	- 9. 99 5	1.00	110.52
	1681	C	ASN A	21	9.915	28.409	-6.547	1.00	81.05
	1682	0	ASN A	21	10.054	29.521	-6.035	1.00	81.05
10	1683	N	VAL A	22	9.681	27.306	- 5.848	1.00	79.17
10	1684	CA	VAL A	22	9.525	27.341	-4.404	1.00	79.17
	1685	CB	VAL A	22	8.057	27.304	-4.012	1.00	85.34
	1686	CG1	VAL A	22	7.431	26.001	-4.486	1.00	85.34
	1687	CG2	VAL A	22	7.925	27.449	-2.510	1.00	85.34
	1688	Ç	VAL A	22	10.194	26.117	-3.815	1.00	79.17
15	1689	0	VAL A	22	10.247	25.070	-4.469	1.00	79.17
	1690	N	THR A	23	10.676	26.240	-2.579	1.00	92.04
	1691	CA	THR A	23	11.367	25.145	-1.908	1.00	92.04
	1692	CB	THR A	23	12.775	25.585	-1.556	1.00	153.40
	1693	OG1	THR A	23	13.414	26.089	-2.736	1.00	153.40
20	1694	CG2	THR A	23	13.567	24.428	-0.993	1.00	153.40
	1695	С	THR A	23	10.667	24.698	-0.634	1.00	92.04
	1696	0	THR A	23	10.364	25.525	0.212	1.00	92.04
	1697	N	LEU A	24	10.403	23.404	-0.485	1.00	64.92
	1698	CA	LEU A	24	9.742	22.945	0.730	1.00	64.92
25	1699	CB	LEU A	24	8.564	22.015	0.427	1.00	83.07
	1700	CG	LEU A	24	7.676	22.301	-0.774	1.00	83.07
	1701	CD1	LEU A	24	6.400	21.482	-0.676	1.00	83.07
	1702	CD2	LEU A	24	7.348	23.745	-0.837	1.00	83.07
	1703	· C	LEU A	24	10.701	22.206	1.657	1.00	64.92
30	1704	O	LEU A	24	11.034	21.049	1.433	1.00	64.92
	1705	N	THR A	25	11.125	22.863	2.725	1.00	
	1706	CA	THR A	25	12.026	22.227	3.665	1.00	60.46
	1707	CB	THR A	25	12.890	23.286	4.309	1.00	60.46
	1708	OG1	THR A	25	13.523	24.040	3.273	1.00	96.68
35	1709	CG2	THR A	25	13.943	22.654	5.175		96.68
	1710	c	THR A	25	11.264	21.446	4.746	1.00 1.00	96.68
	1711	ŏ	THR A	25	10.270	21.923	5. 29 3	1.00	60.46
	1712	Ň	CYS A	26	11.717	20.239	5.048	1.00	60.46
	1713	CA	CYS A	26	11.060	19.464	6.081	1.00	126.10
40	1714	Č	CYS A	26	11.617	19.884	7.421	1.00	126.10
	1715	ŏ	CYS A	26	12.813	20.108	7.566		126.10
	1716	СВ	CYS A	26	11.293	17.971	5.888	1.00	126.10
	1717	SG	CYS A	26	10.283	16.954	7.005	1.00	188.87
	1718	Ň	ASN A	27	10.233	19.999	8.393	1.00	188.87
45	1719	ĊA	ASN A	27	11.065	20.379		1.00	248.12
	1720	CB	ASN A	27	10.474	20.379 19.354	9.747	1.00	248.12
	1721	ČĞ	ASN A	27	10.331		10.685	1.00	249.30
	1722	OD1	ASN A	27	9.999	19.883	12.046	1.00	249.30
	1723	ND2	ASN A	27		21.050	12.192	1.00	249.30
50	1724	C	ASN A	27 27	10.582 12.549	19.060	13.069	1.00	249.30
50	1725	ŏ	ASN A	27 27	13.220	20.546	10.040	1.00	248.12
	1726	Ň	GLY A			19.591	10.431	1.00	248.12
	1727	CA	GLY A	28 28	13.058	21.754	9.840	1.00	150.98
	1728	Č	GLY A		14.469	22.013	10.073	1.00	150.98
55	1729	ŏ		28	14.771	23.413	9.596	1.00	150.98
33	1730	N	GLY A ASN A	28	14.541	23.731	8.435	1.00	150.98
	1731	CA	ASN A	29	15.288	24.258	10.480	1.00	168.28
	1732	CB		29	15.576	.638 نے	10.111	1.00	168.28
	1733		ASN A	29	15.714	26.494	11.374	1.00	185.34
60	1734	CG CD1	ASN A	29	15.723	27.979	11.072	1.00	185.34
w		OD1	ASN A	29	15.387	28.400	9.9 6 6	1.00	185.34
	1735	ND2	ASN A	29	16.097	28.782	12.059	1.00	185.34
	1736	C	ASN A	29	16.799	25.839	9.208	1.00	168.28
	1737	0	ASN A	29	16.704	26.492	8.165	1.00	168.28
65	1738	N O	ASN A	30	17.943	25.279	9.594	1.00	244.43
UJ	1739	CA	ASN A	30	19.151	25.453	8.797	1.00	244.43
	1740	CB	ASN A	30	20.131	26.363	9.543	1.00	249.25
	1741	CG	ASN A	30	19.592	27.765	9.735	1.00	249.25
	1742	OD1	ASN A	30	19.601	28.297	10.843	1.00	249.25
70	1743	ND2	ASN A	30	19.122	28.372	8.654	1.00	249.25
70	1744	С	ASN A	30	19.863	24.172	8.412	1.00	244.43

	1745	0	ASN A	30	19.859	23.770	7.252	1.00	244.43
	1746	N	PHE A	31	20.478	23.527	9.386	1.00	249.41
	1747	CA	PHE A	31	21.210	22.326	9.077	1.00	249.41
_	1748	СВ	PHE A	31	22.639	22,474	9.586	1.00	249.46
5	1749	CG	PHE A	31	23.362	23.675	9.073	1.00	
	1750	CD1	PHE A	31	23.138	24.925	9.634	1.00	249.46
	1751	CD2	PHE A	31	24.250	23.563	8.008	1.00	249.46
	1752	CE1	PHE A	31	23.798	26.050	9.152	1.00	249.46
	1753	CE2	PHE A	31	24.917	24.682	7.514	1.00	249.46
10	1754	CZ	PHE A	31	24.682	25.931	8.083	1.00	249.46
	1755	C	PHE A	31	20.559	21.049	9.617		249.46
	1756	Ö	PHE A	31	20.226	20.949	10.807	1.00	249.41
	1757	Ň	PHE A	32	20.393	20.077		1.00	249.41
	1758	CA	PHE A	32	19.790		8.715	1.00	249.47
15	1759	CB	PHE A	32	18.496	18.777	9.021	1.00	249.47
	1760	CG	PHE A	32	17.642	18.614	8.228	1.00	246.45
	1761	CD1	PHE A			17.487	8.707	1.00	246.45
	1762	CD2	PHE A	32	17.048	17.548	9.963	1.00	246.45
	1763	CE1	PHE A	32	17.442	16.359	7.921	1.00	246.45
20	1764	CE2	PHE A	32	16.272	16.499	10.437	1.00	246.45
20	1765	CZ		32	16.665	15.302	8.387	1.00	248.45
	1766		PHE A	32	16.077	15.378	9.652	1.00	246.45
		C	PHE A	32	20.742	17.630	8.674	1.00	249.47
	1767	0	PHE A	32	21.773	17.852	8.051	1.00	249.47
25	1768	N	GLU A	33	20.392	16.403	9.058	1.00	249.57
25	1769	CA	GLU A	33	21.260	15.270	8.763	1.00	249.57
	1770	CB	GLU A	33	21.850	14.696	10.034	1.00	249.41
	1771	CG	GLU A	33	22.893	13.655	9.727	1.00	249.41
	1772	CD	GLU A	33	24.0 96	14.255	9.017	1.00	249,41
20	1773	OE1	GLU A	33	24.471	15.388	9.373	1.00	249.41
30	1774	OE2	GLU A	33	24.695	13.581	8.140	1.00	249.41
	1775	С	GLU A	33	20.671	14.104	7.992	1.00	249.57
	1776	0	GLU A	33	21.232	13.684	6.982	1.00	249.57
	1777	N	VAL A	34	19.566	13.554	8.485	1.00	216.78
25	1778	CA	VAL A	34	18.961	12.405	7.832	1.00	216.78
35	1779	CB	VAL A	34	17.623	12.017	8.499	1.00	196.07
	1780	CG1	VAL A	34	17.008	10.816	7.801	1.00	196.07
	1781	CG2	VAL A	34	17.864	11.683	9.958	1.00	196.07
	1782	С	VAL A	34	18.754	12.609	6.338	1.00	216.78
40	1783	0	VAL A	34	18.550	13.729	5.860	1.00	216.78
40	1784	N	SER A	35	18.845	11.506	5.608	1.00	172.95
	1785	CA	SER A	35	18.669	11.506	4.170	1.00	172.95
	1786	CB	SER A	35	19.837	10.789	3.489	1.00	249.26
	1787	OG	SER A	35	19.822	9.399	3.775	1.00	249.26
4.5	1788	С	SER A	35	17.368	10.770	3.873	1.00	172.95
45	1789	0	SER A	35	16.978	10.632	2.715	1.00	172.95
	1790	N	SER A	36	16.706	10.290	4.926	1.00	142.42
	1791	CA	SER A	36	15.437	9.579	4.773	1.00	142.42
	1792	CB	SER A	36	15.404	8.320	5.643	1.00	183.21
	1793	OG	SER A	36	15.320	8.643	7.020	1.00	
50	1794	C	SER A	S .7.	14.288	10.498	5.168	1.00	183,21 142,42
	1795	0	SER A	36	13.906	10.585	6.337	1.00	142.42
	1796	N	THR A	37	13.749	11.189	4.171	1.00	
	1797	CA	THR A	37	12.645	12.117			91.48
	1798	CB	THR A	37	13.088	13.579	4.370 4.085	1.00 1.00	91.48
55	1799	OG1	THR A	37	14.193	13.929	4.928		110.07
	1800	CG2	THR A	37	11.960	14.535	4.352	1.00	110.07
	1801	С	THR A	37	11.582	11.689		1.00	110.07
	1802	0	THR A	37	11.902	11.294	3.366 2.244	1.00	91.48
	1803	N	LYS A	38	10.321	11.748		1.00	91.48
60	1804	CA	LYS A	38	9.233	11.345	3.769	1.00	121.21
	1805	СВ	LYS A	38	8.339		2.886	1.00	121.21
	1806	CG	LYS A	38	9.088	10.344	3.600	1.00	152.68
	1807	CD	LYS A	38		9.131	4.112	1.00	152.68
	1808	CE	LYS A	38	8.151	8.168	4.824	1.00	152.68
65	1809	NZ	LYS A	38	8.877 7.952	6.909	5.245	1.00	152.68
	1810	C	LYS A	38	7.952	5.951	5.893	1.00	152.68
	1811	ŏ	LYS A		8.389	12.529	2.442	1.00	121.21
	1812	Ň	TRP A	38 30	8.140	13.440	3.226	1.00	121.21
	1813	ČA	TRP A	39 30	7.954	12.517	1.185	1.00	102.82
70	1814	CB	TRP A	39 30	7.119	13.592	0.656	1.00	102.82
			TENE A	39	7.861	14.401	-0.401	1.00	80.70

			TRP A	20	9.037	15.167	0.113	1.00	80.70
	1815	CG		39					
	1816	CD2	TRP A	39	9.022	16.295	0.994	1.00	80.70
	1817	CE2	TRP A	39	10.366	16.677	1.201	1.00	80.70
	1818	CE3	TRP A	39	8.002	17.015	1.634	1.00	80.70
_						14.922	-0.168	1.00	80.70
5	1819	CD1	TRP A	39	10.351				
	1820	NE1	TRP A	39	11.154	15.826	0.484	1.00	80.70
	1821	CZ2	TRP A	39	10.717	17.745	2.011	1.00	80.70
			TRP A	39	8.355	18.082	2.443	1.00	80.70
	1822	CZ3							
	1823	CH2	TRP A	39	9.703	18.438	2.623	1.00	80.70
10	1824	С	TRP A	39	5.875	13.008	0.026	1.00	102.82
10		ŏ	TRP A	39	5.956	12.079	-0.765	1.00	102.82
	1825						0.368	1.00	
	1826	N	PHE A	40	4.724	13.562			102.87
	1827	CA	PHE A	40	3.489	13.049	-0.175	1.00	102.87
	1828	СВ	PHE A	40	2.633	12.434	0.936	1.00	104.88
15		ČĞ	PHE A	40	3.319	11.346	1.706	1.00	104.88
13	1829								
	1830	CD1	PHE A	40	4.222	11.655	2.715	1.00	104.88
	1831	CD2	PHE A	40	3.050	10.011	1.438	1.00	104.88
	1832	CE1	PHE A	40	4.847	10.652	3.448	1.00	104.88
						8.999	2.167	1.00	104.88
	1833	CE2		40	3.672				
20	1834	CZ	PHE A	40	4.570	9.321	3.174	1.00	104.88
	1835	С	PHE A	40	2.676	14.104	-0.898	1.00	102.87
	1836	ŏ	PHE A	40	1.808	14.741	-0.302	1.00	102.87
						14.287	-2.184	1.00	73.61
	1837	N	HIS A	41	2.952				
	1838	CA	HIS A	41	2.205	15.252	-2.984	1.00	73.61
25	1839	CB	HIS A	41	2.986	15.552	-4.254	1.00	81.93
25		ČĞ	HIS A	41	2.304	16.514	-5.162	1.00	81.93
	1840								
	1841	CD2	HIS A	41	2.173	16.521	-6.507	1.00	81.93
	1842	ND1	HIS A	41	1.661	17.645	-4.706	1.00	81.93
	1843	CE1	HIS A	41	1.158	18.309	-5.731	1.00	81.93
20					1.455	17.648	-6.837	1.00	81.93
30	1844	NE2		41					
	1845	С	HIS A	41	0.811	14.687	-3.318	1.00	73.61
	1846	0	HIS A	41	0.690	13.733	-4.088	1.00	73.61
	1847	N	ASN A	42	-0.234	15.280	-2.740	1.00	96.75
			ASN A		-1.617	14.822	-2.940	1.00	96.75
~~	1848	CA		42					
35	1849	CB	ASN A	42	-2.017	14.809	-4.435	1.00	98.09
	1850	CG	ASN A	42	-2.244	16.205	-5.004	1.00	98.09
	1851	OD1	ASN A	42	-1.466	17.108	-4.726	1.00	98.09
				42	-3.284	16.385	-5.814	1.00	98.09
	1852	ND2	ASN A						
	1853	С	ASN A	42	-1.771	13.413	-2.374	1.00	96.75
40	1854	0	ASN A	42	-2.625	12.652	-2.826	1.00	9 6.75
	1855	N	GLY A	43	-0.948	13.068	-1.386	1.00	89.87
				43	-1.019	11.739	-0.789	1.00	89.87
	1856	ÇA	GLY A						
	1857	С	GLY A	43	-0.054	10.730	-1.410	1.00	89.87
	1858	0	GLY A	43	0.542	9.901	-0.714	1.00	89.87
45	1859	Ñ	SER A	44	0.097	10.798	-2.728	1.00	129.29
73					0.990	9.904	-3,449	1.00	129.29
	1860	CA	SER A	44					
	1861	СВ	SER A	44	0.833	10.113	-4.96 0	1.00	173.89
	1862	OG	SERA	44	-0.521	10.004	-5.358	1.00	173.89
	1863	C	SER A	44	2.436	10.182	-3.043	1.00	129.29
50					2.890	11.322	-3.095	1.00	129.29
50	1864	0	SER A	44					
	1865	N	LEU A	45	3.15 9	9.142	-2.639	1.00	128.43
	1866	CA	LEU A	45	4.559	9.291	-2.239	1.00	128.43
		CB	LEU A	45	5.149	7.925	-1.874	1.00	210.08
	1867						-1.397	1.00	210.08
	1868	CG	LEU A	45	6.602	7.911			
55	1869	CD1	LEU A	45	6.768	8.881	-0.237	1.00	210.08
	1870	CD2	LEU A	45	6.995	6.495	-0.980	1.00	210.08
	1871	Č	LEU A	45	5.379	9.921	-3.365	1.00	128.43
							-4.540	1.00	128.43
	1872	0	LEU A	45	5.129	9.671			
	1873	N	SER A	46	6.354	10.749	-3.007	1.00	150.05
60	1874	CA	SER A	46	7.200	11.403	-4.006	1.00	150.05
			SER A	46	7.500	12.846	-3.588	1.00	129.32
	1875	CB							129.32
	1876	OG.	SER A	46	8.251	13.516	-4.586	1.00	
	1877	C	SER A	46	8.499	10.623	-4.127	1.00	150.05
	1878	Ŏ	SER A	46	8.801	9.796	-3.275	1.00	150.05
65		Ň	GLU A	47	9.274	10.881	-5.177	1.00	207.01
UJ	1879								207.01
	1880	CA	GLU A	47	10.534	10.168	-5.357	1.00	
	1881	СВ	GLU A	47	10.798	9.896	-6.851	1.00	249.57
	1882	CG	GLU A	47	9.574	9.479	-7.672	1.00	249.57
		CD	GLU A	47	9.801	9.602	-9.185	1.00	249.57
~~	1883								
70	1884	OE1	GLU A	47	9.668	10.722	-9.729	1.00	249.57

	1885 1886	OE2 C	GLU A GLU A	47 47	10.133 11.743	8.577 10.894	-9.821 -4.739	1.00 1.00	249.57 207.01
	1887	ŏ	GLU A	47	12.856	10.373	-4.796	1.00	207.01
	1888	N	GLU A	48	11.556	12.084	-4.163	1.00	127.05
5	1889	CA	GLU A	48	12.703	12.760	-3.542	1.00	127.05
	1890	CB	GLU A	48	12.524	14.292	-3.489	1.00	182.29
	1891	CG	GLU A	48	13.615	15.057	-2.682	1.00	182.29
	1892	CD	GLU A	48	15.017	15.011	-3.296	1.00	182.29
	1893	OE1	GLU A	48	15.226	15.631	-4.359	1.00	182.29
10	1894	OE2	GLU A	48	15.914	14.360	-2.713 -2.126	1.00	182.29
	1895	C	GLU A	48	12.882	12.208 11.681	-1.531	1.00 1.00	127.05 127.05
	1896	0	GLU A THR A	48 49	11.938 14.099	12.305	-1.600	1.00	86.20
	1897	N CA	THR A	49	14.385	11.817	-0.258	1.00	86.20
15	1898 1899	CB	THR A	49	15.263	10.549	-0.313	1.00	133.36
13	1900	OG1	THR A	49	16.473	10.832	-1.027	1.00	133.36
	1901	CG2	THR A	49	14.513	9.419	-1.021	1.00	133.36
	1902	Č	THR A	49	15.074	12.903	0.583	1.00	86.20
	1903	Ö	THR A	49	14.950	12 938	1.810	1.00	86.20
20	1904	N ·	ASN A	50	15.787	13.801	-0.085	1.00	156.26
	1905	CA	ASN A	50	16.465	14.888	0.610	1.00	156.26
	1906	CB	ASN A	50	17.158	15.810	-0.406	1.00	185.93
	1907	CG .	ASN A	50	18.159	16.752	0.245	1.00	185.93
25	1908	OD1	ASN A	50	18.105	16.970	1.452 -0.549	1.00 1.00	185.93 185.93
25	1909	ND2	ASN A ASN A	50 50	19.062 15.393	17.323 15.656	1.382	1.00	156.26
	1910	C	ASN A	50 50	14.238	15.689	0.976	1.00	156.26
	1911 1912	Ň	SER A	51	15.765	16.264	2.499	1.00	124.65
	1913	CA	SER A	51	14.804	17.019	3.296	1.00	124.65
30	1914	CB	SER A	51	15.434	17.440	4.628	1.00	124.86
-	1915	ÖĞ	SER A	51	16.427	18.441	4.450	1.00	124.86
	1916	C	SER A	51	14.281	18.263	2.569	1.00	124.65
	1917	0	SER A	51	13.257	18.823	2.959	1.00	124.65
	1918	N	SER A	52	14.979	18.704	1.525	1.00	90.69
35	1919	CA	SER A	52	14.553	19.884	0.780	1.00	90.69
	1920	CB	SER A	52	15.708	20.872	0.631	1.00	131.83
	1921	og .	SER A	52	16.109	21.377	1.894 -0.584	1.00 1.00	131.83 90.69
	1922	C	SER A SER A	52 52	14.038 14.803	19.478 19.073	-1.449	1.00	90.69
40	1923 1924	0 N	LEU A	53	12.727	19.584	-0.756	1.00	92.73
70	1925	ČA	LEU A	53	12.057	19.239	-2.005	1.00	92.73
	1926	CB	LEU A	53	10.720	18.547	-1.710	1.00	96.57
	1927	ČĠ	LEU A	53	9.633	18.561	-2.788	1.00	96.57
	1928	CD1	LEU A	53	10.226	18.224	-4.145	1.00	96.57
45	1929	CD2	LEU A	53	8.536	17.571	-2.396	1.00	96.57
	1930	С	LEU A	53	11.814	20.486	-2.847	1.00	92.73
	1931	0	LEU A	53	10.874	21.231	-2.601	1.00	92.73
	1932	N	ASN A	54	12.660	20.710	-3.846	1.00	74.24
50	1933	CA	ASN A	54	12.508	21.879 22.180	-4.708 -5.442	1.00 1.00	74.24 143.36
50	1934	CB CG	ASN A ASN A	54 54	13.819 14.883	22.734	-4.526	1.00	143.36
	1935 1936	OD1	ASN A	54	14.670	23.738	-3.853	1.00	143.36
	1937	ND2	ASN A	54	16.040	22.086	-4.497	1.00	143.36
	1938	C	ASN A	54	11.390	21.731	-5.727	1.00	74.24
55	1939	ō	ASN A	54	10.937	20.633	-6.038	1.00	74.24
	1940	N	iLE A	55	10.936	22.868	-6.233	1.00	93.23
	1941	CA	ILE A	55	9.898	22.911	-7.249	1.00	93.23
	1942	CB	ILE A	55	8.542	23.323	-6.659	1.00	75.25
	1943	CG2	ILE A	55	7.629	23.783	-7.751	1.00	75.25
60	1944	CG1	ILE A	55	7.932	22.135	-5.918 5.000	1.00	75.25
	1945	CD1	ILE A	55 55	6.605	22.397 23.951	-5.286 -8.241	1.00 1.00	75.25 93.23
	1946	C	ILE A ILE A	, 5 5 55	10.359 10.593	25.100	-7.866	1.00	93.23
	1947 1948	Ň	VAL A	56	10.553	23.543	-9.491	1.00	114.64
65	1949	CA	VAL A	56	10.977	24.469	-10.515	1.00	114.64
55	1950	CB	VAL A	56	12.025	23.820	-11.419	1.00	202.78
	1951	CG1	VAL A	56	12.782	24.892	-12.183	1.00	202.78
	1952	CG2	VAL A	56	12.983	22.997	-10.579	1.00	202.78
	1953	C	VAL A	56	9.771	24.909	-11.333	1.00	114.64
70	1954	0	VAL A	56	8.649	24.730	-10.883	1.00	114.64

			4011 4		. 0.000	25.480	-12.516	1.00	86.89
	1955	N.	ASN A	57	9.993		-13.366	1.00	86.89
	1956	CA	ASN A	57	8.902	25.961	-14.832	1.00	
	1957	СВ	ASN A	57	9.187	25.646			171.09
	1958	CG	ASN A	57	10.333	26.468	-15.379	1.00	171.09
5	1959	OD1	ASN A	57	10.332	27.695	-15.277	1.00	171.09
-	1960	ND2	ASN A	57	11.318	25.799	-15.962	1.00	171.09
	1961	C	ASN A	57	7.549	25.397	-12.962	1.00	86.89
	1962	ŏ	ASN A	57	7.112	24.377	-13.473	1.00	86.89
		N	ALA A	58	6.893	26.087	-12.036	1.00	98.74
10	1963			58	5.610	25.665	-11.500	1.00	98.74
10	1964	CA	ALA A			26.705	-10.525	1.00	108.16
	1965	CB	ALA A	58	5.094		-12.548	1.00	98.74
	1966	C	ALA A	58	4.557	25.376			
	1967	0	ALA A	58	4.185	26.242	-13.327	1.00	98.74
	1968	N	LYS A	59	4.082	24.140	-12.560	1.00	74.98
15	1969	CA	LYS A	59	3.039	23.725	-13.482	1.00	74.98
	1970	СВ	LYS A	59	3.424	22.395	-14,146	1.00	178.83
	1971	ÇĞ	LYS A	59	4.740	22.455	-14.920	1.00	178.83
	1972	CD	LYS A	59	5.158	21.095	-15.463	1.00	178.83
		C.E	LYS A	59	6.483	21.185	-16.215	1.00	178.83
20	1973		LYS A	59	6.932	19.856	-16.725	1.00	178.83
20	1974	NZ			1.782	23.569	-12.623	1.00	74.98
	1975	Č	LYS A	59		23.163	-11.463	1.00	74.98
	1976	0	LYS A	59	1.878				60.66
	1977	N	PHE A	60	0.614	23.912	-13.166	1.00	
	1978	CA	PHE A	60	-0.640	23.780	-12.418	1.00	60.66
25	1979	CB	PHE A	- 60	-1.815	23.834	-13.371	1.00	124.29
	1980	CG	PHE A	60	-1.949	25.140	-14.046	1.00	124.29
	1981	CD1	PHE A	60	-2.524	25.234	-15.301	1.00	124.29
	1982	CD2	PHE A	60	-1.510	26.294	-13.425	1.00	124.29
		CE1	PHE A	60	-2.653	26.464	-15.942	1.00	124.29
30	1983	CE2	PHE A	60	-1.630	27.527	-14.054	1.00	124.29
30	1984			60	-2.209	27.613	-15.313	1.00	124.29
	1985	cz	PHE A			22.496	-11.595	1.00	60.66
	1986	Ç	PHE A	60	-0.714		-10.504	1.00	60.66
	1987	0	PHE A	60	-1.287	22.487		1.00	94.84
	1988	N	GLU A	61	-0.124	21.418	-12.112		
35	1989	CA	GLU A	61	-0.129	20.123	-11.433	1.00	94.84
	1990	СВ	GLU A	61	0.502	19.037	-12.312	1.00	214.43
	1991	CG	GLU A	61	-0.208	18.784	-13.625	1.00	214.43
	1992	CD	GLU A	61	-0.246	20.011	-14.508	1.00	214.43
	1993	OE1	GLU A	61	0.831	20.583	-14.781	1.00	214.43
40		OE2	GLU A	61	-1.352	20.403	-14.930	1.00	214.43
40	1994		GLU A	61	0.626	20.165	-10.114	1.00	94.84
	1995	C			0.397	19.318	-9.253	1.00	94.84
	1996	0	GLU A	61			-9.959	1.00	76.23
	1997	N	ASP A	62	1.535	21.130			76.23
	1998	CA	ASP A	62	2.303	21.242	-8.728	1.00	
45	1999	СВ	ASP A	62	3.493	22.175	-8.913	1.00	161.53
	2000	CG	ASP A	62	4.380	21.755	-10.072	1.00	161.53
	2001	OD1	ASP A	62	4.571	20.536	-10.273	1.00	161.53
	2002	OD2	ASP A	62	4.897	22.644	-10.778	1.00	161.53
	2003	C	ASP A	62	1.407	21.732	-7.614	1.00	76.23
50	2004	ŏ	ASP A	62	1.721	21.544	-6.451	1.00	76.23
50			SER A	63	0.280	22,341	-7.977	1.00	83.22
	2005	N		63	-0.680	22.828	-6.992	1.00	83.22
	2006	CA	SER A			·	-7.691	1.00	115.03
	2007	CB	SER A	63	-1.880	23.464		1.00	115.03
	2008	OG	SER A	63	-1.503	24.633	-8.399		
55	2009	C	SER A	63	-1.140	21.621	-6.212	1.00	83.22
	2010	0	SER A	63	-1.508	20.640	-6.814	1.00	83.22
	2011	N	GLY A	64	-1.124	21.660	-4.887	1.00	65.94
	2012	CA	GLY A	64	-1.575	20.488	-4.154	1.00	65.94
	2013	C	GLY A	64	-1.306	20.493	-2.661	1.00	65. 94
60		ŏ	GLY A	64	-0.942	21.530	-2.082	1.00	65.94
JU	2014		GLU A	65	-1.509	19.337	-2.032	1.00	82.22
	2015	N				19.159	-0.605	1.00	82.22
	2016	CA	GLU A	65 65	-1.285		-0.031	1.00	143.82
	2017	CB	GLU A	65	-2.463	18.376			143.82
,	2018	CG	GLU A	65	-2.304	17.897	1.394	1.00	143.82
65	2019	CD	GLU A	65	-3.356	16.866	1.773	1.00	
	2020	OE1	GLU A	65	-3.374	15.779	1.157	1.00	143.82
	2021	OE2	GLU A	65	-4.169	17.139	2.681	1.00	143.82
	2022	C	GLU A	65	0.035	18.378	-0.420	1.00	82.22
	2023	ŏ	GLU A	65	0.207	17.313	-1.011	1.00	82.22
70	2024	Ň	TYR A	66	0.971	18.903	0.374	1.00	76.24
70	2024	14	1111 7	JJ		. 3.222			

						40.004	0.614	1.00	70.04
	2025	CA	TYR A	66	2.240	18.224			76.24
	2026	CB	TYR A	66	3.377	19.083	0.150	1.00	67.69
	2027	CG	TYR A	66	3.426	19.339	-1.314	1.00	67.69
			TYR A	66	2.574	20.255	-1.915	1.00	67.69
_	2028	CD1							
5	2029	CE1	TYR A	66	2.680	20.572	-3.265	1.00	67.69
	2030	CD2	TYR A	66	4.385	18.724	-2.095	1.00	67.69
	2031	CE2	TYR A	66	4.502	19.017	-3.447	1.00	67.69
				-		19.948	-4.032	1.00	67.69
	2032	CZ	TYR A	66	3.647				
	2033	OH	TYR A	66	3.792	20.230	-5.378	1.00	67.69
10	2034	С	TYR A	66	2.490	17.934	2.083	1.00	76.24
10			TYR A	66	1.891	18.570	2.941	1.00	76.24
	2035	0							
	2036	N	LYS A	67	3.398	17.000	2.375	1.00	93.48
	2037	CA	LYS A	67	3.756	16.664	3.759	1.00	93.48
	2038	CB	LYS A	67	2.619	15.924	4.439	1.00	143.97
15			LYS A		2.079	14.788	3.619	1.00	143.97
15	2039	CG		67					
	2040	CD	LYS A	67	0.876	14.176	4.291	1.00	143.97
	2041	CE	LYS A	67	0.213	13.163	3.385	1.00	143.97
	2042	NZ	LYS A	67	-1.009	12.616	4.023	1.00	143.97
					5.011	15.818	3.806	1.00	93.48
	2043	С		67					
20	2044	0	LYS A	67	5.357	15.166	2.824	1.00	93.48
	2045	N	CYS A	68	5.715	15.852	4.932	1.00	71 <i>.</i> 26
	2046	CA	CYS A	68	6.914	15.044	5.067	1.00	71.26
					6.823	14.232	6.340	1.00	71.26
	2047	Ç	CYS A	68					
	2048	0	CYS A	68	6.020	14.540	7.208	1.00	71.26
25	2049	CB	CYS A	68	8.183	15.905	5.041	1.00	93.73
23	_	SG	CYS A	68	8.385	17.184	6.305	1.00	93.73
	2050						6.425	1.00	106.93
	2051	N	GLN A	69	7.619	13.174			
	2052	CA	GLN A	69	7.651	12.302	7.591	1.00	106.93
	2053	CB	GLN A	69	6.558	11.233	7.476	1.00	95.79
30		CG	GLN A	69	6.744	10.032	8.390	1.00	95.79
30	2054			-					95.79
	2055	CD	GLN A	69	5.702	8.954	8.161	1.00	
	2056	OE1	GLN A	69	5.476	8.521	7.024	1.00	95.79
	2057	NE2	GLN A	69	5.060	8.509	9.244	1.00	95.79
		C	GLN A	69	9.015	11.641	7.629	1.00	106.93
25	2058						6.594	1.00	106.93
35	2059	0	GLN A	69	9.657	11.496			
	2060	N	HIS A	70	9.462	11.243	8.813	1.00	174.41
	2061	CA	HIS A	70	10.753	10.589	8.928	1.00	174.41
	2062	CB	HIS A	70	11.601	11.296	9.977	1.00	160.27
							9.572	1.00	160.27
	2063	CG	HIS A	70	12.022	12.673			
40	2064	CD2	HIS A	70	11.502	13.885	9.873	1.00	1 60.27
	2065	ND1	HIS A	70	13.085	12.909	8.726	1.00	160.27
	2066	CE1	HIS A	70	13.203	14.210	8.527	1.00	160.27
						14.824	9.213	1.00	160.27
	2067	NE2	HIS A	70	12.257				
	2068	С	HIS A	70	10.632	9.112	9.268	1.00	174.41
45	2069	0	HIS A	70	9.543	8.536	9.237	1.00	174.41
	2070	N	GLN A	71	11.764	8.505	9.590	1.00	242.81
							9.923	1.00	242.81
	2071	CA	GLN A	71	11.815	7.091			
	2072	CB	GLN A	71	13.246	6.724	10.335	1.00	199.62
	2073	CG	GLN A	71	13.632	5.293	9.992	1.00	199.62
50	2074	CD	GLN A	71	13.345	4.945	8.543	1.00	199.62
50							7.634	1.00	199.62
	2075	OE1	GLN A	71	14.015	5.423			
	2076	NE2	GLN A	71	12.331	4.115	8.324	1.00	199.62
	2077	С	GLN A	71	10.817	6.722	11.027	1.00	242.81
	2078	Ö	GLN A	71	9.989	5.829	10.844	1.00	242.81
E E						7.419	12.160	1.00	160.50
55	2079	N _.	GLN A	72	10.886				
	2080	CA	GLN A	72	9.991	7.143	13.289	1.00	160.50
	2081	CB	GLN A	72	10.803	6.584	14.465	1.00	249.38
	2082	CG	GLN A	72	9.972	6.150	15.671	1.00	249.38
								1.00	249.38
	2083	CD	GLN A	72	10.819	5.563	16.791	1.00	
60	2084	OE1	GLN A	72	11.537	4.581	16.594	1.00	249.38
	2085	NE2	GLN A	72	10.738	6.164	17.975	1.00	249.38
	2086	Ċ	GLN A	72	9.237	8.392	13.740	1.00	160.50
								1.00	160.50
	2087	0	GLN A	72	9.319	8. 79 7	14.901		
	2088	N	VAL A	73	8.493	9.001	12.825	1.00	139.31
65	2089	CA	VAL A	73	7.759	10.217	13,154	1.00	139.31
-	2090	CB	VAL A	73	8.575	11.467	12.795	1.00	182.81
								1.00	182.81
	2091	CG1	VAL A	73	7.960	12.688	13.430		
	2092	CG2	VAL A	73	10.000	11.297	13.237	1.00	182.81
	2093	С	VAL A	73	6.445	10.284	12.391	1.00	139,31
70	2094	ŏ	VAL A	73	6.352	9.819	11.254	1.00	139.31
10	205	-	4 Che C		0.002	3.313	,,,		

	2095	N	ASN A	74	5.428	10.864	13.019	1.00	98.24
	2096	CA	ASN A	74	4.136	10.988	12.376	1.00	98.24
	2097	CB	ASN A	74	3.045	11.209	13.427	1.00	227.24
	2098	CG	ASN A	74	3.039	10.124	14.489	1.00	227.24
5	2099	QD1	ASN A	74	3.176	8.940	14.170	1.00	227.24
_	2100	ND2	ASN A	74	2.875	10.520	15.748 11.378	1.00 1.00	227.24 98.24
	2101	С	ASN A	74	4.194	12.144	11.700	1.00	98.24
	2102	0	ASN A	74	4.649	13.246 11.863	10.157	1.00	124.76
	2103	N	GLU A	75	3.750	12.842	9.074	1.00	124.76
10	2104	CA	GLU A	75 75	3.730 2.881	12.302	7.921	1.00	249.33
	2105	CB	GLU A	75 75	1.709	11.440	8.364	1.00	249.33
	2106	CG	GLU A GLU A	75 75	1.032	10.734	7.202	1.00	249.33
	2107	CD OE1	GLU A	75	1.730	10.023	6.446	1.00	249.33
15	2108 2109	OE2	GLU A	75	-0.198	10.888	7.048	1.00	249.33
13	2110	Č	GLU A	75	3.245	14.232	9.499	1.00	124.76
	2111	ō	GLU A	75	2.346	14.372	10.327	1.00	124.76
	2112	N	SER A	76	3.859	15.255	8.912	1.00	84.02 84.02
	2113	CA	SER A	76	3.569	16.653	9.208 8.509	1.00 1.00	92.60
20	2114	CB	SER A	76	4.578	17.534 17.395	7.108	1.00	92.60
	2115	og	SER A	76	4.391	17.096	8.754	1.00	84.02
	2116	C	SER A	76 76	2.201 1.599	16.468	7.888	1.00	84.02
	2117	0	SER A	76 77	1.722	18.198	9.323	1.00	82.56
25	2118	N	GLU A GLU A	77 77	0.415	18.751	8.960	1.00	82.56
25	2119	CA CB	GLU A	77	0.413	19.918	9.883	1.00	211.53
	2120	CG	GLU A	77	-0.157	19.511	11.331	1.00	211.53
	2121 2122	CD	GLU A	77	-1.343	18.579	11.512	1.00	211.53
	2123	OE1	GLU A	77	-1.831	18.020	10.505	1.00	211.53
30	2124	OE2	GLU A	77	-1.780	18.396	12.668	1.00	211.53
-	2125	C	GLU A	77	0.550	19.239	7.533	1.00	82.56 82.56
	2126	0	GLU A	77	1.397	20.102	~7. 25 2 6. 60 4	1.00 1.00	57.51
	2127	N	PRO A	78	-0.250	18.679 17.493	6.808	1.00	210.77
	2128	CD	PRO A	78 70	-1.105 -0.226	19.047	5,186	1.00	57.51
35	2129	CA	PRO A	78 70	-0.226 -1.469	18.370	4.644	1.00	210.77
	2130	CB	PRO A PRO A	78 78	-1.440	17.076	5.376	1.00	210.77
	2131	CG C	PRO A	78	-0.193	20.544	4.936	1.00	57.51
	2132 2133	ŏ	PRO A	78	-0.607	21.338	5.785	1.00	57.51
40	2134	Ň	VAL A	79	0.343	20.931	3.789	1.00	75.93
40	2135	ĊA	VAL A	79	0.396	22.331	3.422	1.00	75.93
	2136	CB	VAL A	79	1.780	22.859	3.574	1.00 1.00	49.48 49.48
	2137	CG1	VAL A	79	1.916	24.215	2.850 5.039	1.00	49.48
	2138	ÇG2	VAL A	79	2.078	23.010 22.466	1.972	1.00	75.93
45	2139	C	VAL A	79 70	-0.033 0.463	21.748	1.113	1.00	75.93
	2140	0	VAL A TYR A	79 80	-0.961	23.375	1.696	1.00	60.67
	2141	N CA	TYR A	80	-1.424	23.519	0.336	1.00	60.67
	2142 2143	CB	TYR A	80	2.903	23.814	0.280	1.00	249.12
50	2143	ČG	TYR A	80	-3.420	23.538	-1.115	1.00	249.12
50	2145	CD1	TYR A	80	-3.434	22.256	-1.623	1.00	249.12
	2146	CE1	TYR A	80	-3.870	22.005	-2.920	1,00	249.12 249.12
	2147	CD2	TYR A	80	-3.902	24.575	-1.927	1.00 1.00	249.12 249.12
	2148	CE2	TYR A	80	-4.414	24.332	-3.216 -3.703	1.00	249.12
55	2149	cz	TYR A	80	-4.378	23.015	-4.929	1.00	249.12
	2150	ÓН	TYR A	80	-4.926 -0.736	22.722 24.582	-0.438	1.00	30.67
	2151	C	TYR A	80 80	-0.736 -0.537	25.688	0.043	1.00	60.67
	2152	0	TYR A LEU A	81	-0.414	24.264	-1.669	1.00	53.62
60	2153 2154	N CA	LEU A	81	0.237	25.227	-2.520	1.00	53.62
UU	2155	CB	LEU A	81	1.547	24.619	-3.003	1.00	66.18
	2156	cG	LEU A	81	2.237	25.486	-4.035	1.00	66.18
	2157	CD1	LEU A	81	2.603	26.806	-3.373	1.00	66.18
	2158	CD2	LEU A	81	3.461	24.803	-4.566	1.00	66.18
65	2159	С	LEU A	81	-0.703	25.487	-3.698	1.00	53.62 53.62
	2160	0	LEU A	81	-1.229	24.534	-4.283 -4.048	1.00 1.00	63.15
	2161	N	GLU A	82	-0.956	26.742 26.990	-4.048 -5.201	1.00	63.15
	2162	CA	GLU A	82	-1.821 -3.099	26.890 27.700	-4.772	1.00	149.46
-	2163	CB CC	GLU A	82 82	-3.0 9 9 -4.259	27.463	-5.722	1.00	149.46
70	2164	CG	GLU A	QZ.	7.2.00	21.700			

	2165	CD	GLU A	82	-5.537	28.157	-5.276	1.00	149.46
	2166	OE1	GLU A	82	-5.798	28.194	-4.050	1.00	149.46
	2167	OE2	GLU A	82	-6.286	28.653	-6.151	1.00	149.46
_	2168	Ç	GLU A	82	-1.100	27.823 28.878	-6.283 -5.996	1.00 1.00	63.15 63.15
5	2169	0	GLU A VAL A	82 83	-0.503 -1.157	28.876 27.352	-7.526	1.00	58.52
	2170	N CA	VAL A	83	-0.517	28.050	-8.632	1.00	58.52
	2171 2172	CB	VAL A	83	0.194	27.083	-9.516	1.00	61.79
	2173	CG1	VAL A	83	0.749	27.819	-10.728	1.00	61.79
10	2174	CG2	VAL A	83	1.294	26.427	-8.738	1.00	61.7 9
	2175	Ċ	VAL A	83	-1.473	28.859	-9.501	1.00	58.52
	2176	0	VAL A	83	-2.540	28.364	-9.877	1.00 1.00	58.52 70.51
	2177	N	PHE A	84	-1.082	30.088 30.947	-9.839 -10.632	1.00	70.51 70.51
1.5	2178	CA	PHE A	84 84	-1.947 -2.395	30.947 32.164	-9.834	1.00	69.94
15	2179	CB CG	PHE A PHE A	84	-2.395 -3.130	31.836	-8.588	1.00	69.94
	2180 2181	CD1	PHE A	84	-2.455	31.374	-7.488	1.00	69.94
	2182	CD2	PHE A	84	-4.503	32.031	-8.498	1.00	69.94
	2183	CE1	PHE A	84	-3.134	31.108	-6.323	1.00	69.94
20	2184	CE2	PHE A	84	-5.199	31.764	-7.324	1.00	69.94
	2185	CZ	PHE A	84	-4.521	31.312	-6.242	1.00	69.94 70.51
	2186	C	PHE A	84	-1.390	31.480 31.452	-11.923 -12.179	1.00 1.00	70.51 70.51
	2187	0	PHE A	84	-0.186 -2.327	31.985	-12.717	1.00	86.88
25	2188	N GA	SER A SER A	85 85	-2.327 -2.067	32.625	-13.989	1.00	86.88
25	2189 2190	CB	SER A	85	-2.453	31.714	-15.142	1.00	135.23
	2191	OG OG	SER A	85	-2.214	32.358	-16.378	1.00	135.23
	2192	Č	SER A	85	-2.999	33.835	-13.959	1.00	86.88
	2193	Ö	SER A	85	-4.226	33.670	-14.007	1.00	86.88
30	2194	N	ASP A	86	-2.425	35.033	-13.836	1.00	47.41 47.41
	2195	CA	ASP A	86	-3.209	36.256 36.259	-13.803 -12.589	1.00 1.00	131.95
	2196	CB	ASP A	86 86	-4.131 -5.454	36.927	-12.876	1.00	131.95
	2197	CG OD1	ASP A ASP A	86 86	-5.433	38.087	-13.345	1.00	131.95
35	2198 2199	OD2	ASP A	86	-6.509	36.296	-12.629	1.00	131.95
23	2200	C	ASP A	86	-2.245	37.453	-13.756	1.00	47.41
	2201	ŏ	ASP A	86	-1.043	37.284	-13.502	1.00	47.41
	2202	N	TRP A	87	-2.760	38.661	-14.004	1.00	62.18 62.18
	2203	CA	TRP A	87	-1.903	39.848	-14.009	1.00 1.00	225.09
40	2204	CB	TRP A	87	-2.668	41.090 41.233	-14.457 -15.914	1.00	225.09
	2205	CG	TRP A	87 87	-2. 632 -3.596	40.723	-16.830	1.00	225.09
	2206	CD2 CE2	TRP A	87	-3.100	40.950	-18.122	1.00	225.09
	2207 2208	CE3	TRP A	87	-4.834	40.077	-16.683	1.00	225.09
45	2209	CD1	TRP A	87	-1.618	41.757	-16.666	1.00	225.09
	2210	NE1	TRP A	87	-1.891	41.586	-17.994	1.00	225.09
	2211	CZ2	TRP A	87	-3.794	40.549	-19.261	1.00	225.09
	2212	CZ3	TRP A	87	-5.528	39.687	-17.820	1.00 1.00	225.09 225.09
	2213	CH2	TRP A	87	-5.008 -1.350	39.923 40.068	-19.086 -12. 64 5	1.00	62,18
50	2214	C	TRP A	87 87	-1.350 -0.139	40.149	-12.468	1.00	62.18
	2215 2216	0 N	LEU A	88	-2.249	40.140	-11.673	1.00	74.08
	2217	GA	LEU A	88	-1.863	40.372	-10.295	1.00	74.08
	2218	CB	LEU A	88	-2.457	41.681	-9.805	1.00	87.26
55	2219	CG	LEU A	88	-1.907	42.914	-10.492	1.00	87.26
	2220	CD1	LEU A	88	-2.496	44.139	-9.837	1.00	87.26
	2221	CD2	LEU A	88	-0.394	42.908	-10.383 -9.369	1.00 1.00	87.26 74.08
	2222	Ç	LEU A	88	-2.305 -3.399	39.274 38.723	-9.501	1.00	74.08
۲0	2223	0	LEU A LEU A	88 89	-3.38 8 -1.456	38.978	-8.399	1.00	49.26
60	2224 2225	N CA	LEU A	89	-1.769	37.943	-7.432	1.00	49.26
	2225 2226	CB	LEU A	89	-0.902	36.718	-7.675	1.00	70.28
	2227	ÇĞ	LEU A	89	-1.170	35.653	-6. 637	1.00	70.28
	2228	CD1	LEU A	89	-2.692	35.436	-6.511	1.00	70.28
65	2229	CD2	LEU A	89	-0.455	34.401	-7.046	1.00	70.28
	2230	Ç	LEU A	89	1.499	38.470	-6.036 5.794	1.00	49.26 49.26
	2231	0	LEU A	89	-0.429	39.008 38.343	-5.784 -5.127	1.00 1.00	72.68
	2232	N	LEU A	90	-2.459 -2.240	38.342 38.815	-3.127 -3.760	1.00	72.68
70	2233 2234	CA CB	LEU A	90 90		39.231	-3.111	1.00	33.75
70	المراجعة المراجعة	~	A		,				

	2235	CG	LEU A	90	-3.444	39.630 40.814	-1.648 -1.620	1.00 1.00	33.75 33.75
	2236	CD1 CD2	LEU A	90 90	-2.488 -4.790	40.011	-1.047	1.00	33.75 33.75
	2237 2238	C	LEU A	90	-1.623	37.701	-2.931	1.00	72.68
5	2239	ŏ	LEU A	90	-2.254	36.674	-2.710	1.00	72.68
	2240	Ň	GLN A	91	-0.398	37.896	-2.462	1.00	48.17
	2241	CA	GLN A	91	0.255	ଅମ.864	-1.656	1.00	48.17
	2242	CB	GLN A	91	1.692	36.682	-2.110	1.00	50.84
10	2243	CG	GLN A	91	1.773	36.315	-3.559 2.071	1.00	50.84
10	2244	CD	GLN A	91	3.159	35.954 36.801	-3.971 -4.013	1.00 1.00	50.84 50.84
	2245	OE1 NE2	GLN A GLN A	91 91	4.041 3.371	34.688	-4.271	1.00	50.84 50.84
	2246 2247	C	GLN A	91	0.218	37.151	-0 165	1.00	48.17
	2248	ŏ	GLN A	91	0.282	38.298	0. 254	1.00	48.17
15	2249	Ň	ALA A	92	0.098	36.113	0.648	1.00	56.37
	2250	CA	ALA A	92	0.044	36.326	80ن.2	1.00	56.37
	2251	СВ	ALA A	92	-1.329	36.039	2.579	1.00	37.31
	2252	. С	ALA A	92	1.033	35.422	2.769	1.00	56.37
	2253	0	ALA A	92	1.202	24.266	2.381	1.00	56.37
20	2254	N	SER A	93	1.695	35. 939	3.794 4.535	1.00	55.78 55.78
	2255	CA	SER A	93	2.665	35.146 35.909	4.535 5.763	1.00 1.00	55.78 74.91
	2256	CB OG	SER A SER A	93 93	3.171 2.111	36.461	6.531	1.00	74.91
	2257 2258	C	SER A	93	1.912	33.019	4.956	1.00	55.78
25	2259	ŏ	SER A	93	2.205	32.828	4.501	1.00	55.78
23	2260	Ň	ALA A	94	0.904	34.112	5.796	1.00	63.55
	2261	CA	ALA A	94	0.070	33.021	6.287	1.00	63.55
	2262	СВ	ALA A	94	0.410	32.712	7.734	1.00	137.30
	2263	С	ALA A	94	-1.392	33.445	6.162	1.00	63.55
30	2264	0	ALA A	94	-1.713	34.616	6.341	1.00	63.55
	2265	N	GLU A	95	-2.283	32.501	5.856	1.00	58.25
	2266	CA	GLU A	95	-3.702	32.826	5.684 4.701	1.00	58.25 138.90
	2267	CB	GLU A	95 05	-4.344 -3.695	31.866 31.890	3.337	1.00 1.00	138.90
35	2268	CG CD	GLU A	95 9 5	-3.695 -4.541	31.214	2.269	1.00	138.90
22	2269 2270	OE1	GLU A	95 ·	-4.085	31.137	1.108	1.00	138.90
	2271	OE2	GLU A	95	-5.664	30.763	2.584	1.00	138.90
	2272	č_	GLU A	95	-4.494	32.844	6.979	1.00	58.25
	2273	Ŏ	GLU A	95	-5.600	33.381	7.016	1.00	58.25
40	2274	N	VAL A	96	-3.934	32.267	8.040	1.00	62.67
	2275	CA	VAL A	96	-4.584	32.253	9.353	1.00	62.67
	2276	CB	VAL A	96	-5.180	30.912	9.637	1.00	62.13 62.13
	2277	CG1	VAL A	96 06	-6.169 -5.835	31.021 30.401	10.762 8.402	1.00 1.00	62.13
45	2278 2279	CG2 C	VAL A VAL A	96 96	-3.512	32.568	10.386	1.00	62.67
40	2280	ŏ	VAL A	96	-2.422	31.999	10.335	1.00	62.67
	2281	Ň	VAL A	97	-3.829	33.449	11.333	1.00	50.85
	2282	CA	VAL A	97	-2.833	33.902	12.289	1.00	50.55
	2283	CB	VAL A	97	-2.307	35.276	11.860	1.00	70.57
50	2284	CG1	VAL A	97	-1.069	35.609	12.633	1.00	70.57
	2285	CG2	VAL A	97	-2.063	35.319	10.372	1.00	70.57
	2286	Ç	VAL A	97	-3.285 -4.373	34.077 34.653	13. 723 13.953	1.00 1.00	50.85 50.85
	2287	0	VAL A	97 98	-4.373 -2.449	33.629	14.673	1.00	73.49
55	2288 2289	N CA	MET A MET A	98	-2.749	33.780	16.096	1.00	73.49
33	2290	CB	MET A	98	-1.766	32.956	16.916	1.00	226.40
	2291	ČĞ	MET A	98	-1.855	31.478	16.645	1.00	228.45
	2292	SD	MET A	98	-3.227	30.766	17.530	1.00	228.45
	2293	CE	MET A	98	-2.529	30.766	19.195	1.00	228.45
60	2294	Ç	MET A	98	-2.617	35.276	16.477	1.00	73.49
	2295	o	MET A	98	-1.636	35.921	16.109	1.00 1.00	73.49 97.63
	2296	N	GLU A	99	-3.595 3.546	35.826	17.202 17.603	1.00	97.63
	2297	CA	GLU A	99	-3.546 4.552	37.228 37.499	18.710	1.00	188.19
65	2298 2299	CB CG	GLU A GLU A	99 99	-4.562 -4.954	37.489 38.958	18.826	1.00	188.19
O.J	2399	CD	GLU A	99	-5.707	39.259	20.106	1.00	188.19
	2301	Œ1	GLU A	99	-6.524	38.412	20.529	1.00	188.19
	2302	OE2	GLU A	99	-5.492	40.347	20.682	1.00	188.19
	2303	С	GLU A	99	-2.146	37.510	18.128	1.00	97.63
70	2304	0	GLU A	99	-1.651	36.783	18.987	1.00	97.63

	2305	N	GLY A	100	-1.492	38.538	17.594	1.00	88.99
	2306 2307	CA C	GLY A GLY A	100 100	-0.159 0.992	38.881 38.577	18.066 17.130	1.00 1.00	88.99 88.99
	2308	ŏ.	GLY A	100	2.071	39.135	17.293	1.00	88.99
5	2309	Ň	GLN A	101	0.777	37.699	16.154	1.00	57.71
	2310	CA	GLN A	101	1.820	37.329	15.192	1.00	57.71
	2311	CB	GLN A	101	1.568	35.933	14.652	1.00	91.13
	2312 2313	CG CD	GLN A GLN A	101 101	1.663 2.932	34.861 34.976	15.708 16.532	1.00 1.00	91.13 91.13
10	2314	OE1	GLN A	101	3.038	35.828	17.420	1.00	91.13
	2315	NE2	GLN A	101	3.912	34.131	16.230	1.00	91.13
	2316	Ç	GLN A	101	1.973	38.281	14.017	1.00	57.71
	2317 2318	0 N	GLN A PRO A	101 102	1.117 3.070	39.124 38.153	13.763 13.266	1.00 1.00	57.71 72.70
15	2319	CD	PRO A	102	4.201	37,220	13.403	1.00	73.79 74.96
15	2320	CA	PRO A	102	3.264	39.049	12.130	1.00	73.79
	2321	СВ	PRO A	102	4.760	38.932	11.873	1.00	74.96
	2322	ÇG	PRO A	102	5.018	37.499	12.139	1.00	74.96
20	2323 2324	C O	PRO A PRO A	102 102	2.425 2.053	38.610 37.446	10.940 10.831	1.00 1.00	73.79 73.70
20	2325	N	LEU A	103	2.125	39.551	10.054	1.00	73.79 77.13
	2326	ĈA	LEU A	103	1.345	39.258	8.862	1.00	77.13
	2327	СВ	LEU A	103	-0.101	39.627	9.094	1.00	77.95
25	2328	CG	LEU A	103	-0.892	39.326	7.831	1.00	77.95
25	2329 2330	CD1 CD2	LEU A LEU A	103 103	-0.843 -2.324	37.836 39. 79 9	7.584 7.975	1.00 1.00	77.95 77.95
	2331	C	LEU A	103	1.850	40.060	7. 68 0	1.00	77.13
	2332	ŏ	LEU A	103	1.892	41.280	7.769	1.00	77.13
•	2333	N	PHE A	104	2.226	39.404	6.580	1.00	65.06
30	2334	CA	PHE A	104	2.708	40.147	5.410	1.00	65.06
	2335 2336	CB CG	PHE A PHE A	104 104	4.175 5.118	39.821 40.096	5.102 6.246	1.00 1.00	119.06 119.06
	2337	ÇD1	PHE A	104	5.209	39.208	7.312	1.00	119.06
	2338	CD2	PHE A	104	5.926	41.237	6.255	1.00	119.06
35	2339	CE1	PHE A	104	6.086	39.443	8.379	1.00	119.06
	2340	CE2	PHE A	104	6.811	41.486	7.321	1.00	119.06
	2341 2342	CZ C	PHE A PHE A	104 104	6.891 1.869	40.585 39.886	8.382 4.164	1.00 1.00	119.06 65.06
	2343	ŏ	PHE A	104	1.640	38.741	3.816	1.00	65.06
40	2344	N	LEU A	105	1.373	40.944	3.519	1.00	48.39
	2345	CA	LEU A	105	0.597	40.795	2.282	1.00	48.39
	2346 2347	CB CG	LEU A LEU A	105 105	-0.708 -1.516	41.544 41.145	2.354 3.570	1.00 1.00	38.52 38.52
	2348	CD1	LEU A	105	-2.952	41.785	3. 5 15	1.00	38.52
45	2349	CD2	LEU A	105	-1.587	39.647	3.571	1.00	38.52
	2350	Ç	LEU A	105	1.445	41.417	1.205	1.00	48.39
	2351	0	LEU A	105	2.137	42.397	1.461	1.00	48.39
	2352 2353	N CA	ARG A ARG A	106 106	1.385 2.198	40.872 41.394	0.001 -1.074	1.00 1.00	64.12 64.12
50	2354	CB	ARG A	106	3.424	40.501	-1.232	1.00	100.28
	2355	CG	ARG A	106	4.313	40.873	-2.370	1.00	100.28
	2356	CD	ARG A	106	5.351	39.801	-2.607	1.00	100.28
	2357	NE	ARG A	106	6.190	40.124	-3.755	1.00	100.28
55	2358 2359	CZ NH1	ARG A ARG A	106 106	6.892 6.854	39. 234 37. 9 57	-4.443 -∕100	1.00 1.00	100,28 100,28
33	2360	NH2	ARC 4	106	7.619	39.623	-5.484	1.00	100.28
	2361	C	ARG A	106	1.416	41.451	-2.380	1.00	64.12
	2362	0	ARG A	106	0.842	40,444	-2.799	1.00	64.12
60	2363	N	CYS A	107	1.349	42.619	-3.018	1.00	99.13
w	2364 2365	CA C	CYS A CYS A	107 107	0.651 1.710	42.685 42.307	-4.301 -5.317	1.00 1.00	99.13 99.13
	2366	ŏ	CYS A	107	2.639	43.059	-5. 5 75	1.00	99.13
	2367	CB	CYS A	107	0.113	44.075	-4.597	1.00	103.70
C E	2368	sg	CYS A	107	-1.146	44.090	-5.916	1.00	103.70
65	2369	N	HIS A	108	1.573	41.112 40.575	-5.868 6.804	1.00	72.29 72.20
	2370 2371	CA CB	HIS A HIS A	108 108	2.530 2.799	40.575 39.131	-6.804 -6.429	1.00 1.00	72.29 116.05
	2372	ČĠ	HIS A	108	3.921	38.508	-7.191	1.00	116.05
	2373	CD2	HIS A	108	3.973	37.391	-7.950	1.00	116.05
70	2374	ND1	HIS A	108	5.195	39.028	-7.190	1.00	116.05

	2375	CE1	HIS A	108	5.986	38.256	-7.913	1.00	116.05
	2376	NE2	HIS A		5.268	37.255	-8.385	1.00	116.05
	2377	Ç .	HIS A		2.119	40.651	-8 <i>.</i> 271	1.00	72.29
5	2378	0	HIS A		1.045	40.176	-8.674	1.00	72 <u>.29</u>
,	2379 2380	N CA	GLY A		2.999 2.735	41.242 41.367	-9.070 -10.485	1.00	118.98
	2381	č	GLY A		3.202	40.136	-10.485 -11.231	1.00 1.00	118.98
	2382	ō	GLY A		4.083	39.410	-10.772	1.00	11 8.9 8 118.98
	2383	N	TRP A		2.603	39.894	-12.389	1.00	106.09
10	2384	CA	TRP A		2.968	38.751	-13.202	1.00	106.09
	2385	CB	TRP A		2.016	38.629	-14.395	1.00	134.90
	2386 2387	CG CD2	TRP A		2.418	37.581	-15.361	1.00	134.90
	2388	CE2	TRP A		1.980 2.657	36.223 35.576	-15.380	1.00	134.90
15	2389	CE3	TRP A		1.072	35.481	-16.431 -14.604	1.00 1.00	134.90 134.90
	2390	CD1	TRP A		3.314	37.707	-16.370	1.00	134.90
	2391	NE1	TRP A		3.466	36.509	-17.021	1.00	134.90
	2392	CZ2	TRP A		2.464	34.224	-16.732	1.00	134.90
20	2393	CZ3	TRP A		0.879	34.132	-14.905	1.00	134.90
20	2394 2395	CH2 C	TRP A		1.575	33.521	-15.958	1.00	134.90
	2396	ŏ	TRP A		4.399 4.916	38.899 40.008	-13.683 -13.825	1.00 1.00	106.09
	2397	Ň	ARG A		5.043	37.764	-13.918	1.00	106.09 87.25
	2398	CA	ARG A		6.426	37.750	-14.392	1.00	87.25
25	2399	CB	ARG A		6.468	38.086	-15.858	1.00	235.25
	2400	CG	ARG A		6.316	36.881	-16.692	1.00	235.25
	2401	CD NE	ARG A		6.642	37.245	-18.072	1.00	235.25
	2402 2403	NE CZ	ARG A		7.428	36.197	-18.691	1.00	235.25
30	2404	NH1	ARG A		8.674 9.295	35.887 36.552	-18.358 -17. 39 2	1.00 1.00	235.25 235.25
50	2405	NH2	ARG A		9.290	34.895	-18.988	1.00	235.25
	2406	C	ARG A		7.358	38.697	-13.665	1.00	87.25
	2407	0	ARG A		8.402	39.105	-14.191	1.00	87.25
35	2408	N	ASN A		6.964	39.048	-12.453	1.00	105.23
33	2409 2410	CA CB	ASN A		7.744	39.942	-11.633	1.00	105.23
	2410	CG	ASN A		9.121 9.735	39.353 39.907	-11. 37 5 -10.118	1.00 1.00	116.08
	2412	OD1	ASN A		9.369	41.000	-10.118 -9.660	1.00	116.08 116.08
	2413	ND2	ASN A		10.668	39.166	-9.544	1.00	116.08
40	2414	С	ASN A		7.905	41.345	-12.218	1.00	105.23
	2415	0	ASN A		8.852	42.055	-11.885	1.00	105.23
	2416	N	TRP A		6.992	41.753	-13.089	1.00	124.66
	2417 2418	CA CB	TRP A		7.095 6.019	43.088 43.344	-13.645	1.00	124.66
45	2419	Ğ	TRP A		6.315	43.344 42.730	-14.688 -15.979	1.00 1.00	167.38 167.38
	2420	CD2	TRP A		5.379	42.134	-16.868	1.00	167.38
	2421	CE2	TRP A		6.091	41.718	-18.006	1.00	167.38
	2422	CE3	TRP A		3.997	41.914	-16.816	1.00	167.38
50	2423	CD1	TRP A		7.533	42.658	-16.592	1.00	167.38
50	2424 2425	NE1 CZ2	TRP A		7.406 5.475	42.049	-17.813	1.00	167.38
	2426	CZ3	TRP A		3.383	41.093 41.293	-19.080 -17.886	1.00 1.00	167.38 167.38
	2427	CH2	TRP A		4.126	40.886	-19.004	1.00	167.38
	2428	C	TRP A		6.939	44.106	-12.540	1.00	124.66
55	2429	0	TRP A	113	6.964	43.768	-11.357	1.00	124.66
	2430	N	ASP A		6.773	45.359	-12.937	1.00	183.63
	2431	CA CB	ASP A		6.603	46.430	-11.981	1.00	183.83
	2432 2433	CG	ASP A		7.598 8.978	47.558 47.269	-12.258	1.00	145.30
60	2434	OD1	ASP A		9.077	47.087	-11. 69 2 -10. 45 9	1.00 1.00	145.30 145.30
	2435	OD2	ASP A		9.957	47.225	-12.473	1.00	145.30
	2436	С	ASP A	114	5.188	46.956	-12.034	1.00	183.83
	2437	0	ASP A	114	4.598	47.106	-13.108	1.00	183.83
65	2438	N	VAL A		4.645	47.216	-10.853	1.00	117.62
O)	2439 2440	CA CB	VAL A		3.294	47.740 46.825	-10.735	1.00	117.62
	2441	CG1	VAL A		2.421 0.971	46.835 47.248	-9.879 -10.008	1.00 1.00	77.28 77.28
	2442	CG2	VAL A		2.616	45.40 9	-10.006 -10.302	1.00	77.28 77.28
	2443	С	VAL A		3.329	49.116	-10.089	1.00	117.62
70	2444	0	VAL A		4.142	49.377	-9.191	1.00	117.62

	0445		7D/D 4						
	2445	N	TYR A	116	2.444	49.995	-10.553	1.00	77.55
	2446	CA	TYR A	116	2.380	51.344	-10.021	1.00	77.55
	2447	CB	TYR A	116	2.831	52.352	-11.086	1.00	167.00
5	2448	CG	TYR A	116	4.271	52.172	-11.532	1.00	167.00
,	2449	CD1	TYR A	116	4.581	51.453	-12.676	1.00	167.00
	2450	CE1	TYR A	116	5.909	51.265	-13.071	1.00	167.00
	2451 2452	CD2 CE2	TYR A TYR A	116	5.325 6.653	52.793	-10.789	1.00	167.00
	2453	CZ	TYR A	116 116	6.937	52.519	-11.173	1.00	167.00
10	2454	OH	TYR A	116	8.246	51.800	-12.312	1.00	167.00
10	2455	C	TYR A	116	0.984	51.608 51.600	-12.687	1.00	167.00
	2456	ŏ	TYR A	116	0.023	51.699	-9.519 0.740	1.00	77.55
	2457	Ň	LYS A	117	0.023	50.951 52.842	-9.742 -8.840	1.00	77.55
	2458	ĊA	LYS A	117	-0.399	53.292	-8.310	1.00	94.85
15	2459	CB	LYS A	117	-1.300	53.834	-9.423	1.00 1.00	94.85
	2460	ČĠ	LYS A	117	-1.084	55.291	-9.786	1.00	193.46
	2461	CD	LYS A	117	-2.284	55.824	-10.563	1.00	193.46 193.46
	2462	CE	LYS A	117	-3.569	55.726	-9.735	1.00	193.46
	2463	NZ	LYS A	117	-4.780	56.210	-10.464	1.00	193.46
20	2464	С	LYS A	117	-1.099	52.125	-7.629	1.00	94.85
	2465	0	LYS A	117	-2.226	51.770	-7.977	1.60	94.85
	2466	N	VAL A	118	-0.422	51.530	-6.655	1.00	105.41
	2467	CA	VAL A	118	-0.979	50.402	-5.927	1.00	105.41
25	2468	СВ	VAL A	118	0.122	49.503	-5.445	1.00	73.04
25	2469	CG1	VAL A	118	-0.314	48.777	-4.205	1.00	73.04
	2470	CG2	VAL A	118	º 455	48.521	-6.514	1.00	73.04
	2471	C	VAL A	118	-1.862	50.736	-4.723	1.00	105.41
	2472	0	VAL A	118	-1.527	51.582	-3.894	1.00	105.41
30	2473	N	ILE A	119	-2.971	50.020	-4.607	1.00	71.97
30	2474 2475	CA	ILE A	119	-3.902	50.248	-3.518	1.00	71.97
	2475 2476	CB CG2	ILE A ILE A	119	-5.125	51.002	-4.016	1.00	<i>7</i> 7.41
	2477	CG1	ILE A ILE A	119 119	-6.037 -4.687	51.319 52.285	-2.866	1.00	77.41
	2478	CD1	ILE A	119	-5.804	52.265 52.949	-4.705 -5.4 6 7	1.00 1.00	77.41
35	2479	C	ILE A	119	-4.395	48.928	-2.961	1.00	77.41
	2480	ŏ	ILE A	119	-4.954	48.146	-3.701	1.00	71.97 71.97
	2481	N	TYR A	120	-4.193	48.654	-1.679	1.00	64.29
	2482	CA	TYR A	120	-4.698	47.403	-1.117	1.00	64.29
40	2483	СВ	TYR A	120	-3.867	46.908	0.059	1.00	49.60
40	2484	ca	TYR A	120	-2.521	46.438	-0.297	1.00	49.60
	2485	CD1	TYR A	120	-1.472	47.324	-0.395	1.00	49.60
	2486	CE1	TYR A	120	-0.195	46.897	-0.736	1.00	49.60
	2487 2488	CD2 CE2	TYR A	120	-2.292	45.109	-0.546	1.00	49.60
45	2489	CZ	TYR A TYR A	120	-1.026	44.650	-0.901	1.00	49.60
15	2490	OH	YR A	120 120	0.020 1.2 6 8	45.548 45.005	-0.992	1.00	49.60
	2491	Č.	TYR A	120	-6.069	45.095 47.879	-1.339 -0.580	1.00	49.60
	2492	ŏ	TYR A	120	-6.313	48.764	-0.069	1.00 1.00	64.29
	2493	Ň	TYR A	121	-6.945	46.686	-0.658	1.00	64.29 62.29
50	2494	CA	TYR A	121	-8.299	46.838	-0.154	1.00	62.29
	2495	CB	TYR A	121	-9.315	46.752	-1.302	1.00	87.89
	2496	CG	TYR A	121	-9.308	47.900	-2.293	1.00	87.89
	2497	CD1	TYR A	121	-8.219	48.119	-3.126	1.00	87.89
	2498	CE1	TYR A	121	-8.232	49.147	-4.073	1.00	87.89
55	2499	CD2	TYR A	121	-10.422	48.745	-2.424	1.00	87.89
	2500	CE2	TYR A	121	-10.450	49.776	-3.368	1.00	87.89
	2501	CZ	TYR A	121	-9.351	49.970	-4.193	1.00	3 7.89
	2502	ÓН	TYR A	121	-9.383	50. 96 6	-5.156	1.00	87.89
60	2503	C	TYR A	121	-8.647	45.772	0.883	1.00	62.29
UU	2504 2505	0	TYR A	121	-8.275	44.598	0.723	1.00	62.29
	2506 2506	N CA	LYS A	122	-9.349	46.180	1.943	1.00	53.98
	2507	CB	LYS A	122	-9.794	45.238	2.957	1.00	53.98
	2508	CG	LYS A	122	-9.069	45.436	4.278	1.00	98.53
65	2509	CD	LYS A LYS A	122 122	-9.499 -9.038	44.427	5.329 6.710	1.00	98.53
	2510	CE	LYS A	122	-9.644	44.809 43.912	6.719 7.774	1.00	98.53
	2511	NZ	LYS A	122	-9.317	43.812 44.426	7.774 9.120	1.00 1.00	98.53
	2512	c	LYS A	122	·11.291	45.452	3.158	1.00	98.53 53.98
	2513	0	LYS A	122	-11.720	46.526	3.569	1.00	53.98
70	2514	N	ASP A	123	-12.081	44.429	2.841	1.00	82.84

	•								
	2515	CA	ASP A	123	-13.530	44,491	2.976	1.00	82.84
	2516	CB	ASP A	123	-13.926	44.624	4.449		
		ča						1.00	104.85
	2517		ASP A	123	-13.786	43.313	5.204	1.00	104.85
_	2518	OD1	ASP A	123	-14.244	42.269	4.680	1.00	104.85
5	2519	OD2	ASP A	123	-13.228	43.321	6.324	1.00	104.85
	2520	С	ASP A	123	-14.140	45.620	2.158	1.00	
	2521	ŏ	ASP A	123	-15.013	46.350	2.638		82.84
								1.00	82.84
	2522	N	GLY A	124	-13.677	45.743	0.915	1.00	89.57
	2523	CA	GLY A	124	-14.179	46.772	0.018	1.00	89.57
10	2524	С	GLY A	124	-13.699	48.197	0.279	1.00	89.57
	2525	0	GLY A	124	-13.981	49.093	-0.528	1.00	89.57
	2526	Ň	GLU A	125	-12.978	48.412	1.382		09.37
								1.00	81.16
	2527	CA	GLU A	125	-12.476	49.746	1.745	1.00	81.16
	2528	СВ	GLU A	125	-12.470	49.925	3.274	1.00	176.94
15	2529	CG	GLU A	125	-13.834	49.988	3.958	1.00	176.94
	2530	CD	GLU A	125	-14.499	51.350	3.844	1.00	176.94
	2531	OE1	GLU A	125	-13.931	52.343	4.352		
								1.00	176.94
	2532	OE2	GLU A	125	-15.595	51.428	3.251	1.00	176.94
	2533	С	GLU A	125	-11.055	50.008	1.238	1.00	81.16
20	2534	0	GLU A	125	-10.223	49.116	1.229	1.00	81.16
	2535	N	ALA A	126	-10.772	51.228	0.815	1.00	
	2536								92.74
		CA	ALA A	126	-9.424	51.546	0.375	1.00	92.74
	2537	СВ	ALA A	126	-9.379	52.967	-0.145	1.00	165.28
	2538	С	ALA A	126	-8.592	51.410	1.650	1.00	92.74
25	2539	0	ALA A	126	-9.083	51.719	2.731	1.00	92.74
	2540	Ň	LEU A	127	-7.347	50.957	1.550		
	2541							1.00	58.95
		CA		127	-6.544	50.778	2.749	1.00	58.95
	2542	CB	LEU A	127	-6.333	49.305	3.037	1.00	73.14
	2543	CG	LEU A	127	-6.046	49.150	4.528	1.00	73.14
30	2544	CD1	LEU A	127	-7.224	49.745	5.285	1.00	73.14
	2545	CD2	LEU A	127	-5.840	47.693			
							4.917	1.00	73.14
	2546	Ç	LEU A	127	-5.195	51.457	2.764	1.00	58.95
	2547	0	LEU A	127	-4.910	52.212	3.691	1.00	58.95
	2548	N	LYS A	128	-4.344	51.153	1.788	1.00	77.17
35	2549	CA	LYS A	128	-3.028	51.788	1.690	1.00	77.17
	2550	CB	LYS A	128	-1.920	50.862	2.197		
	2551	CG						1.00	133.78
			LYS A	128	-2.041	50.465	3.656	1.00	133.78
	2552	CD	LYS A	128	-1.716	51.601	4.605	1.00	133.78
	2553	CE	LYS A	128	-1.741	51.120	6.052	1.00	133.78
40	2554	NZ	LYS A	128	-1.293	52.157	7.033	1.00	133.78
	2555	C	LYS A	128	-2.788	52.130	0.212	1.00	77.17
	2556	ŏ	LYS A	128					
					-3.348	51.493	-0.675	1.00	77.17
	2557	N	TYR A	129	-1.973	53.142	-0.063	1.00	64.91
	2558	CA	TYR A	129	-1.693	53.519	-1.444	1.00	64.91
45	2559	CB	TYR A	129	-2.633	54.637	-1.882	1.00	122.39
	2560	CG	TYR A	129	-2.100	55.390	-3.080	1.00	122.39
	2561	CD1	TYR A	129	-2.232	54.874	-4.366	1.00	
	2562	CE1							122.39
			TYR A	129	-1.702	55.539	-5.465	1.00	122.39
	2563	CD2	TYR A	129	-1.416	56.599	-2.919	1.00	122.39
50	2584	CE2	TYR A	129	-0.875	57.273	-4.012	1.00	122.39
	2565	CZ	TYR A	129	-1.024	56.738	-5.282	1.00	122.39
	2566	OH	TYR A	129	-0.508				
		_				57.402	-6.370	1.00	122.39
	2567	C	TYR A	129	-0.244	53.978	-1.679	1.00	64.91
	2568	0	TYR A	129	0.320	54.739	-0.885	1.00	64.91
55	2569	N	TRP A	130	0.348	53.530	-2.787	1.00	121.28
	2570	CA	TRP A	130	1.713	53.914	-3.125	1.00	121.28
	2571	CB	TRP A						
	2071			130	2.715	52.874	-2.627	1.00	194.88
	2572	CG	TRP A	130	2.557	52.464	-1.196	1.00	194.88
	2573	CD2	TRP A	130	3.398	52.848	-0.100	1.00	194.88
60	2574	CE2	TRP A	130	2.909	52.182	1.049	1.00	194.88
	2575	CE3	TRP A	130	4.508	53.694	0.023	1.00	194.88
	2576	CD1							
	20/0		TRP A	130	1.629	51.608	-0.683	1.00	194.88
	2577	NE1	TRP A	130	1.833	51.431	0.666	1.00	194.88
	2578	CZ2	TRP A	130	3.500	52,334	2.309	1.00	194.88
65	2579	CZ3	TRP A	130	5.096	53.847	1.280	1.00	194.88
-	2580	CH2	TRP A	130	4.592	53.163	2.403	1.00	194.88
	2581	C	TRP A						
				130	1.907	54.064	-4.627	1.00	121.28
	2582	0	TRP A	130	1.075	53.627	-5.422	1.00	121.28
=-	2583	N	TYR A	131	3.015	54.685	-5.015	1.00	100.84
70	2584	CA	TYR A	131	3.304	54.849	-6.426	1.00	100.84
					,				.00.04

	2585	CB	TYR A	131	4.202	56.059	-6.683	1.00	400.00
	2586	CG	TYR A	131	4.299	56.369	-8.155	1.00	199.69 199.69
	2587	CD1	TYR A	131	3.223	56.944	-8.830	1.00	199.69
5	2588	CE1	TYR A	131	3.246	57.115	-10.206	1.00	199.69
J	2589 2590	CD2 CE2	TYR A	131 131	5.414 5.448	55.982 56.149	-8.899	1.00	199.69
	2591	CZ	TYR A	131	4.357	56.148 56.712	-10.281 -10.926	1.00 1.00	199.69
	2592	ОH	TYR A	131	4.364	56.843	-12.295	1.00	199.69 199.69
10	2593	С	TYR A	131	4.029	53.572	-6.818	1.00	100.84
10	2594	0	TYR A	131	3.397	52.644	-7.326	1.00	100,84
	2595 2596	N CA	GLU A GLU A	132 132	5.351	53.543	-6.624	1.00	218.16
	2597	CB	GLU A	132	6.122 7.629	52. 331 52. 547	-6.894 -6.666	1.00 1.00	218.16
	2598	ĊĠ	GLU A	132	8.382	53.317	-7.762	1.00	249.55 249.55
15	2599	CD	GLU A	132	9.480	52.482	-8.422	1.00	249.55
	2600	OE1	GLU A	132	9.903	51.469	-7.822	1.00	249.55
	2601 2602	OE2 C	GLU A GLU A	132 132	9.922 5.531	52.848 51.536	-9.533	1.00	249.55
	2603	ŏ	GLU A	132	5.514	52.022	-5.747 -4.616	1.00 1.00	218.16
20	2604	N	ASN A	133	5.032	50.334	-6.012	1.00	218.16 155.99
	2605	CA	ASN A	133	4.388	49.588	-4.939	1.00	155.99
	2606 2607	CB CG	ASN A ASN A	133	3.656	48.353	-5.472	1.00	108.04
	2608	OD1	ASN A	133 133	4.538 5.620	47.157 47.230	-5.575	1.00	108.04
25	2609	ND2	ASN A	133	4.085	46.035	-6.143 -5.035	1.00 1.00	108.04 108.04
	2610	С	ASN A	133	5.244	49.194	-3.759	1.00	155.99
	2611	0	ASN A	133	6.458	49.376	-3.734	1.00	155.99
	2612 2613	N CA	HIS A	134	4.560	48.629	-2.779	1.00	115.35
30	2614	CB	HIS A	134 134	5.153 4.782	48.235 49.305	-1.520 -0.489	1.00	115.35
	2615	ČĠ	HIS A	134	5.436	49.129	0.842	1.00 1.00	200.02 200.02
	2616	CD2	HIS A	134	4.912	48.893	2.067	1.00	200.02
	2617	ND1	HIS A	134	6.799	49.213	1.016	1.00	200.02
35	2618 2619	CE1 NE2	HIS A	134	7.088	49.035	2.293	1.00	200.02
33	2620	C	HIS A	134 134	5.961 4.596	48.840 48.874	2.951 -1.114	1.00 1.00	200.02
	2621	Ö	HIS A	134	4.008	46.161	-1.934	1.00	115.35 115.35
	2622	N	ASN A	135	4.781	46.524	0.153	1.00	81.38
40	2623 2624	CA	ASN A	135	4.298	45. 263 .	0.675	1.00	81.38
TU	2625	CB CG	ASN A ASN A	135 135	5.426 5.832	44.243 43.891	0.654	1.00	168.37
	2626	OD1	ASN A	135	4.964	43.656	-0.754 -1.596	1.00 1.00	168.37 168.37
	2627	ND2	ASN A	135	7.134	43.839	-1.029	1.00	168.37
45	2628	C	ASN A	135	3.748	45.431	2.073	1.00	81.38
43	2629 2630	0	ASN A ILE A	135 136	4.455	45.219	3.042	1.00	81.38
	2631	CA CA	ILE A	136	2.481 1.826	45.817 46.032	2.168 3.456	1.00 1.00	68.07
	2632	CB	ILE A	136	0.288	46.019	3.287	1.00	68.07 £6.88
50	2633	CG2	ILE A	136	-0.135	44.814	2.531	1.00	86.88
3 0	2634 2635	CG1 CD1	ILE A	136	-0.397	46.040	4.638	1.00	86.88
	2636	C	ILE A	136 136	-1.885 2.277	46.136 44.997	4.514	1.00	36.88
	2637	ŏ	ILE A	136	2.085	43.801	4.482 4.301	1.00 1.00	68.07
~ ~	2638	N	SER A	137	2.904	45.484	5.550	1.00	68.07 113.35
55	2639	CA	SER A	137	3.422	44.631	6.606	1.00	113.35
	2640 2641	C8 OG	SER A SER A	137	4.932	44.798	6.686	1.00	. 0.04
	2642	C	SER A	137 137	5. 433 2. 808	44.258 44.903	7.891 7.974	1.00 1.00	73.04
	2643	Ö	SER A	137	2.469	46.029	8.304	1.00	113.35 113.35
60	2644	N	ILE A	138	2.688	43.856	8.777	1.00	71.19
	2645 2646	CA	ILE A	138	2.116	43.961	10.117	1.00	71.19
	2647	CB CG2	ILE A	138 138	0.715	43.413	10.147	1.00	41.44
	2648	CG1	ILE A	138	0.257 -0.212	43.304 44.297	11.582 9.318	1.00 1.00	41.44
65	2649	CD1	ILE A	138	-1.531	43.627	9.019	1.00	41.44 41.44
	2650	C	ILE A	138	2.922	43.170	11.146	1.00	71.19
	2651	0	ILE A	138	3.093	41.954	11.012	1.00	71.19
	2652 2653	N CA	THR A	139 139	3.397	43.856	12.185	1.00	108.53
70	2654	CB	THR A	139	4.195 5.001	43.216 44.260	13.234 14.012	1.00	108.53
•		- -		.00		VV	17.012	1.00	232.49

	2655	OG1	THR A	139	4.127	45.304	14.460	1.00	232.49
	2656	CG2	THR A	139	6.080	44.854	13.121	1.00	232.49
	2657	C	THR A	139	3.291	42.458	14.192	1.00	
	2658	0	THR A	139	3.199	41.235	14.125	1.00	108.53
5	2659	Ñ	ASN A	140	2.632	43.192	15.083		108.53
	2660	CA	ASN A	140	1.699	42.621		1.00	125.42
	2661	CB	ASN A	140	1.662		16.050	1.00	125.42
	2662	CG	ASN A	_		43.455	17.328	1.00	148.98
	2663			140	0.619	42.967	18.305	1.00	148.98
10		OD1	ASN A	140	-0.533	42.738	17.950	1.00	148.98
10	2664	ND2	ASN A	140	1.024	42.828	19.558	1.00	148.98
	2665	С	ASN A	140	0.335	42.677	15.375	1.00	125.42
	2666	0	ASN A	140	-0.149	43.763	15.030	1.00	125.42
	2667	N	ALA A	141	-0.291	41.518	15.203	1.00	57.61
	2668	CA	ALA A	141	-1.569	41.462	14.527	1.00	
15	2869	СВ	ALA A	141	-1.605	40.246	13.644	1.00	57.61
	2670	C	ALA A	141	-2.785	41.468			27.12
	2671	ŏ	ALA A				15.439	1.00	57.61
	2672	Ň		141	-2.895	40.661	16.364	1.00	57.61
			THR A	142	-3.713	42.373	15.149	1.00	70.60
20	2673	CA	THR A	142	-4.939	42.481	15.912	1.00	70.60
20	2674	CB	THR A	142	-5.488	ذ ي 43 .5	15.811	1.00	136.27
	2675	OG1	THR A	142	-4.440	44.833	16.136	1.00	136.27
	2676	CG2	THR A	142	-6.643	44.104	16.773	1.00	136.27
	2677	С	THR A	142	-5.937	41.478	15.334	1.00	
	2678	0	THR A	142	-5.666	40.852	14.311		70.60
25	2679	Ñ	VAL A	143	-7.066	41.285		1.00	70.60
	2680	ĊA	VAL A	143	-8.057		16.001	1.00	71.67
	2681	CB	VAL. A			40.355	15.489	1.00	71.67
				143	-8.949	39.782	16.610	1.00	65.94
	2682	CG1	VAL A	143	-9.785	40.880	17.217	1.00	65.94
20	2683	CG2	VAL A	143	-9.848	38.672	16.047	1.00	65.94
30	2684	С	VAL A	143	-8.934	41.126	14.518	1.00	71.67
	2685	0	VAL A	143	-9.679	40.552	13.726	1.00	71.67
	2686	N	GLU A	144	-8.842	42.442	14.579	1.00	
	2687	CA	GLU A	144	-9.650	43.260	13.699	1.00	71.12
	2688	CB	GLU A	144	-9.747	44.691			71.12
35	2689	ČĠ	GLU A	144	-10.475	44.796	14.235	1.00	228.43
	2690	CD	GLU A				15.566	1.00	228.43
	2691	OE1		144	-9.558	45.204	16.699	1.00	228.43
			GLU A	144	-8.966	46.296	16.611	1.00	228.43
	2692	OE2	GLU A	144	-9.428	44.440	17.676	1.00	228.43
40	2693	Ç	GLU A	144	-9.068	43.250	12.301	1.00	71.12
40	2694	0	GLU A	144	-9.732	43.609	11.338	1.00	71.12
	2695	N	ASP A	145	-7.821	42.820	12.194	1.00	58.24
	2696	CA	ASP A	145	-7.146	42.754	10.900	1.00	58.24
	2697	СВ	ASP A	145	-5.645	42.541	11.091	1.00	
	2698	CG	ASP A	145	-4.945	43.784	11.606		106.20
45	2699	OD1	ASP A	145	-5.013	44.817		1.00	106.20
	2700	OD2	ASP A	145	-4. 32 9		10.911	1.00	106.20
	2701	C	ASP A			43.733	12.696	1.00	106.20
	2702			145	-7.705	41.643	10.018	1.00	58.24
		0	ASP A	145	-7.434	41.608	8.819	1.00	58.24
50	2703	N	SER A	146	-8.490	40.744	10.607	1.00	85.01
3 0	2704	CA	SER A	146	-9.077	39.652	9.848	1.00	85.01
	2705	CB	SER A	146	-9.781	38.669	10.789	1.00	118.46
	2706	OG	SER A	146	-8.854	38.089	11.691	1.00	118.46
	2707	С	SER A	146	-10.052	40.266	8.855		
	2708	0	SER A	146	-10.741	41.227		1.00	85.01
55	2709	Ň	GLY A	147	-10.081		9.168	1.00	85.01
	2710	ĊA	GLY A			39.735	7.644	1.00	64.55
	2711	č		147	-10.972	40.264	6.632	1.00	64.55
			GLY A	147	-10.649	39.664	5.277	1.00	64.55
	2712	0	GLY A	147	-9.963	38.628	5.214	1.00	64.55
<i>ζ</i> Λ	2713	N.	THR A	148	-11.147	40.285	4.201	1.00	54.60
60	2714	ÇA	THR A	148	-10.881	39.795	2.841	1.00	54.60
	2715	CB	THR A	148	-12.159	39.339	2.143	1.00	77.82
	2716	OG1	THR A	148	-12,541	40.316	1.193	1.00	77.82
	2717	CG2	THR A	148	-13.272	39.179	3.148	1.00	
	2718	C	THR A	148	-10.204	40.891			77.82
65	2719	ŏ	THR A	148	-10.789		2.029	1.00	54.60
	2720	Ň	TYR A			41.941	1.746	1.00	54.60
				149	-8.958	40.639	1.661	1.00	38.49
	2721	CA CB	TYR A	149	-8.181	41.622	0.950	1.00	38.49
	2722	CB	TYR A	149	-6.775	41.604	1.518	1.00	47.71
70	2723	ca	TYR A	149	-6.654	41.954	2.987	1.00	47.71
70	2724	CD1	TYR A	149	-7.128	41.123	3.982	1.00	47.71
					*				77.71

	2725 2726 2727	CE1 CD2 CE2	TYR A TYR A TYR A	149 149 149	-6.952 -6.010 -5.832	41.468 43.124 43.470	5.327 3.370 4.691	1.00	47.71 47.71
_	2728	cz ·	TYR A	149	-6.297	42.656	5.669	1.00	47.71
5	2729	ОН	TYR A	149	-6.098	43.066	6.973	1.00 1.00	47.71
	2730	С	TYR A	149	-8.098	41.368	-0.543	1.00	47.71 38.49
	2731	0	TYR A	149	-8.451	40.272	-1.006	1.00	38.49
	2732	N.	TYR A	150	-7.639	42.382	-1.279	1.00	53.38
10	2733 2734	CA	TYR A	150	-7.385	42.305	-2.716	1.00	53.38
10	2734 2735	CB CG	TYR A TYR A	150	-8.681	42.142	-3.520	1.00	86.43
	2736	CD1	TYR A TYR A	150 150	-9.564 0.467	43.353	-3.735	1.00	86.43
	2737	CE1	TYR A	150	-9.167 -9.992	44.393 45.488	-4.563 -4.795	1.00	86.43
	2738	CD2	TYR A	150	-10.816	43.436	-3.142	1.00	86.43
15	2739	CE2	TYR A	150	-11.652	44.522	-3.365	1.00 1.00	86.43 86.43
	2740	CZ	TYR A	150	-11.234	45.547	-4.190	1.00	86.43
	2741	он	TYR A	150	-12.049	46.642	-4.381	1.00	86.43
	2742 2743	C	TYR A	150	-6.653	43.598	-3.028	1.00	53.38
20	2743	N	TYR A CYS A	150	-6.726	44.536	-2.225	1.00	53.38
	2745	ĊA	CYS A	151 151	-5.900 -5.179	43.660 44.894	-4.127	1.00	73.39
	2746	C	CYS A	151	-5.388	45.311	-4.462 -5.900	1.00	73.39
	2747	Ó	CYS A	151	-5.741	44.487	·6.721	1.00 1.00	73.39
25	2748	CB	CYS A	151	-3.680	44.745	-4.197	1.00	73.39 73.27
25	2749	SG	CYS A	151	-2.861	43.358	-5.059	1.00	73.27
	2750	N	THR A	152	-5.177	46.593	-6.192	1.00	98.75
	2751 2752	CA CB	THR A THR A	152	-5.335	47.121	-7.537	1.00	98.75
	2753	001	THR A	152 152	-6.478 -6.138	48.154	-7.602	1.00	109.76
30	2754	CG2	THR A	152	-0.138 -7.746	49.310 47.558	-6.821 -7.048	1.00	109.76
	2755	C	THR A	152	-4.025	47.793	-7.048 -7.905	1.00 1.00	109.76
	2756	0	THR A	152	-3.329	48.322	-7.032	1.00	98.75 98.75
	2757	N _.	GLY A	153	-3.681	47.764	-9.188	1.00	91.16
35	2758 2759	CA	GLY A	153	-2.444	48.385	-9.622	1.00	91.16
55	2760	CO	GLY A GLY A	153	-2.392	48.562	-11.122	1.00	91.16
	2761	Ň	LYS A	153 154	-3.163 -1.488	47.947 49.409	-11.843	1.00	91.16
	2762	ČA	LYS A	154	-1.359	49.409 49.643	-11.597 -13.023	1.00	71.11
40	2763	CB	LYS A	154	-1.229	51.140	-13.299	1.00 1.00	71.11 173.07
40	2764	CG	LYS A	154	-1.235	51.523	-14.769	1.00	173.07
	2765	CD	LYS A	154	-1.155	53.036	-14.911	1.00	173.07
	2766 2767	CE NZ	LYS A	154	-1.050	53.490	-16.359	1.00	173.07
	2768	C	LYS A Lys a	154 154	-0.857 -0.120	54.960	-16.420	1.00	173.07
45	2769	ŏ	LYS A	154	0.963	48.907 49.009	-13.500	1.00	71.11
	2770	N	VAL A	155	-0.289	48.128	-12.900 -14.563	1.00 1.00	71.11
	2771	CA	VAL A	155	0.813	47.372	-15.153	1.00	155.85 155.85
	2772	CB ·	VAL A	155	0.510	45.884	-15.201	1.00	196.06
50	2773	CG1	VAL A	155	1.673	45.144	-15.841	1.00	196.06
50	2774 2775	CG2 C	VAL A VAL A	155	0.273	45.373	-13.809	1.00	196.06
	2776	ŏ	VAL A VAL A	155 155	0.960 -0.013	47.894 47.054	-16.560	1.00	155.85
	2777	Ň	TRP A	156	2.187	47.951 48.251	-17.309	1.00	155.85
	2778	CA	TRP A	156	2.437	48.821	-16.912 -18.215	1.00	136.77
55	2779	CB	TRP A	156	1.888	47.941	-19.308	1.00 1.00	136.77 189.17
	2780	CG	TRP A	156	2.584	46.701	-19.394	1.00	نة با 109.17 نة 9.17
	2781	CD2	TRP A	156	3.991	46.538	-19.596	1.00	169.17
	2782 2783	CE2 CE3	TRP A	156	4.260	45.184	-19.532	1.00	169.17
60	2784	CD1	TRP A	156 156	5.037	47.423	-19.855	1.00	169.17
	2785	NE1	TRP A	156	2.066 3.053	45.478 44.565	-19.202	1.00	169.17
	2786	CZ2	TRP A	156	5.536	44.634	-19.283 -19.734	1.00	169.17
	2787	CZ3	TRP A	156	6.293	46.924	-20.012	1.00 1.00	169.17 169.17
65	2788	CH2	TRP A	156	6.542	45.522	-19.971	1.00	169.17
U)	2789	C	TRP A	156	1.664	50.102	-18.251	1.00	136.77
	2790 2791	O N	TRP A	156	2.130	51.132	-17.775	1.00	136.77
	2792	CA	GLN A GLN A	157 157	0.445	50.004	-18.777	1.00	192.06
	2793	CB	GLN A	157	-0.395 -0.133	51.166 51.791	-18.902	1.00	192.06
70	2794	CG	GLN A	157	1.231	52.449	-20,263 -20,291	1.00 1.00	249.57
								1.00	249.57

	2795	CD	GLN A	157	1.374	53.420	-19.126	1.00	249.57
	2796	OE1	GLN A	157	0.539	54.293	-18.950	1.00	249.57
	2797	NE2	GLN A	157	2.428	53.271	-18.339	1.00	249.57
5	2798 2799	C	GLN A GLN A	157 157	-1.873 -2.717	50.913 51.753	-18.673 -18.989	1.00	192.06
,	2800	Ň	LEU A	158	-2.181	49.753	-18.108	1.00 1.00	192.06 96.98
	2801	CA	LEU A	158	-3.565	49.394	-17.813	1.00	96.98
	2802	· CB	LEU A	158	-4.018	48.234	-18.697	1.00	92.50
10	2803	CG	LEU A	158	-4.362	48.530	-20.148	1.00	92.50
10	2804	CD1 CD2	LEU A	158	-5.577	47.691	-20.496	1.00	92.50
	2805 2806	C	LEU A	158 158	-4.695 -3.758	50.015 49.028	-20.343 -16.345	1.00 1.00	92.50
	2807	ŏ	LEU A	158	-2.821	48.596	-15.661	1.00	96.98 96.98
	2808	N	ASP A	159	-4.983	49.216	-15.869	1.00	119.40
15	2809	CA	ASP A	159	-5.330	48.925	-14.485	1.00	119.40
	2810	CB	ASP A	159	-6.442	49.875	-14.018	1.00	201.99
	2811 2812	CG OD1	ASP A ASP A	159	-6.096	51.345	-14.236	1.00	201.99
	2813	OD2	ASP A	159 159	-5.103 -6.823	51. 832 52.018	-13.651 -15.000	1.00 1.00	201.99
20	2814	C	ASP A	159	-5.793	47.473	-14.334	1.00	201.99 119.40
	2815	O	ASP A	159	-6.417	46.919	-15.235	1.00	119.40
	2816	N	TYR A	160	-5.475	46.860	-13.197	1.00	117.93
	2817	CA	TYR A	160	-5.875	45.481	-12.929	1.00	117.93
25	2818	CB CC	TYR A	160	-4.769	44.503	-13.308	1.00	127.75
23	2819 2820	CG CD1	TYR A	160 160	-4.261 -3,184	44.648 45.483	-14.715	1.00	127.75
	2821	CE1	TYR A	160	-3.164	45.463 45.625	-14.997 -16.277	1.00 1.00	127.75 127.75
	2822	CD2	TYR A	160	-4.855	43.952	-15.766	1.00	127.75
	2823	CE2	TYR A	160	-4.386	44.087	-17.061	1.00	127.75
30	2824	CZ	TYR A	160	-3.309	44.932	-17.297	1.00	127.75
	2825	ОН	TYR A	160	-2.808	45.145	-18.541	1.00	127.75
	2826 2827	C	TYR A	160	-6.239	45.240	-11.471	1.00	117.93
	2828	Ň	TYR A GLU A	160 161	-5.674 -7.184	45.836 44.335	-10.557 -11.275	1.00 1.00	117.93
35	2829	ČA	GLU A	161	-7.665	43.963	-9.960	1.00	99.07 99.07
	2830	CB	GLU A	161	-9.179	44.113	-9.945	1.00	160.66
	2831	CG	GLU A	161	-9 .877	43.683	-8.681	1.00	160.66
	2832	CD	GLU A	161	-11.290	44.226	-8.624	1.00	160.66
40	2833 2834	OE1 OE2	GLU A	161	-12.117	43.690	-7.85 6	1.00	160.66
40	2835	C	GLU A	161 161	-11.564 -7.258	45.206 42.507	-9. 350 -9.699	1.00 1.00	160.66 99.07
	2836	ŏ	GLU A	161	-7.346	41.672	-10.598	1.00	99.07
	2837	N	SER A	162	-6.806	42.206	-8.481	1.00	84.68
	2838	CA	SER A	162	-6.378	40.856	-8.119	1.00	84.68
45	2839	CB	SER A	162	-5.247	40.923	-7.102	1.00	134.29
	2840 2841	og	SER A	162	-5.670	41.599	-5.932	1.00	134.29
	2842	C O	SER A	162 162	-7.520 -8.592	40.029 40.555	-7.536 -7.230	1.00 1.00	84.68
	2843	Ň	GLU A	163	-7.292	38.729	-7.230 -7.382	1.00	84.68 56.84
50	2844	CA	GLU A	163	-8.316	37.829	-6.842	1.00	56.84
	2845	СВ	GLU A	163	-7.885	36.370	-7.015	1.00	162.97
	2846	CG	GLU A	163	-7.984	35.836	-8.438	1.00	162.97
	2847	CD	GLU A	163	-9.417	35.601	-8.869	1.00	162.97
55	2848 2849	OE1 OE2	GLU A	163	-10.122	34.835	-8.175	1.00	162.97
55	2850	C	GLU A	163 163	-9.835 -8.437	36.176 38.151	-9.900 -5.368	1.00 1.00	162.97 56.84
	2851	ŏ	GLU A	163	-7.439	38.433	-4.720	1.00	56.84
	2852	N	PRO A	164	-9.660	38.122	-4.805	1.00	48.99
60	2853	CD	PRO A	164	-10.959	37.760	-5.379	1.00	93.04
60	2854	CA	PRO A	164	-9.789	38.423	-3.371	1.00	48.99
	2855 2856	CB CG	PRO A	164	-11.295	38.547	-3.196	1.00	93.04
	2857	C	PRO A	164 164	-11.814 -9.201	37.544 37.307	-4.135 -2.528	1.00	93.04
•	2858	ŏ	PRO A	164	-9.101	36.160	-2.526 -2.977	1.00 1.00	48.99 48.99
65	2859	Ň	LEU A	165	-8.802	37.625	-1.303	1.00	69.69
	2860	· CA	LEU A	165	-8.236	36.609	-0.426	1.00	69.69
	2861	CB	LEU A	165	-6.733	36.661	-0.465	1.00	37.26
	2862	CG	LEU A	165	-6.041	35.774	0.560	1.00	37.26
70	2863 2864	CD1 CD2	LEU A	165	-6.655	34.407	0.459	1.00	37.26
, 0	2004	CD2	LEU A	165	-4.535	35.665	0.301	1.00	37.26

	0005	•							
	2865 2866	C	LEU A	165	-8.661	36.800	1.000	1.00	69.69
	2867	Ň	ASN A	165 166	-8.430 -9.272	37.863 35.777	1.562 1.585	1.00	69.69
	2868	ČA	ASN A	166	-9.725	35.861	2.962	1.00 1.00	67.70
5	2869	CB	ASN A	166	-10.806	34.849	3.224	1.00	67.70 76.12
	2870	CG	ASN A	166	-12.182	35.396	2.998	1.00	76.12
	2871	OD1	ASN A	166	-12.414	36.571	3.171	1.00	76.12
	2872	ND2	ASN A	166	-13.106	34.519	2.633	1.00	76.12
10	2873 2874	c o	ASN A ASN A	166 166	-8.606 -7. 72 4	35.605	3.943	1.00	67.70
	2875	Ň	ILE A	167	-8.665	34.792 36.273	3.687 5. 0 90	1.00 1.00	67.70
	2876	CA	ILE A	167	-7.634	36.127	6.105	1.00	54.98 54.98
	2877	CB	ILE A	167	-6.686	37.292	6.049	1.00	41.48
15	2878	CG2	ILE A	167	-5. 88 3	37.357	7.277	1.00	41.48
15	2879	CG1	ILE A	167	-5.770	37.131	4.855	1.00	41.48
	2880 2881	CD1 C	ILE A ILE A	167 167	-4.655 -8.248	38.164	4.815	1.00	41.48
	2882	ŏ	ILE A	167	-0.248 -9.113	36.093 36.914	7.478 7.783	1.00 1.00	54.98
	2883	Ň	THR A	168	-7.820	35.163	8.317	1.00	54.98 55.70
20	2884	CA	THR A	168	-8.391	35.122	9.642	1.00	55.70
	2885	CB	THR A	168	-9.241	33.875	9.837	1.00	71.33
	2886	OG1	THR A	168	-10.289	33.866	8.860	1.00	71.33
	2887 2888	CG2 C	THR A	168	-9.857	33.869	11.209	1.00	71.33
25	2889	Ö	THR A THR A	168 168	-7.339 -6.2 9 5	35.171	10.697	1.00	55.70
	2890	Ň	VAL A	169	-7.618	34.539 35.950	10. 587 11. 72 4	1.00 1.00	55.70 64.35
	2891	CA	VAL A	169	-6.725	36.090	12.863	1.00	64.35
	2892	CB	VAL A	169	-6.370	37.560	13.087	1.00	77.36
30	2893	CG1	VAL A	169	-5.895	37.772	14.468	1.00	77.36
30	2894 2895	CG2	VAL A	169	-5.314	37.978	12.128	1.00	77.36
	2896	C	VAL A VAL A	169 169	-7.539 -8.510	35.567 36.203	14.048	1.00	64.35
	2897	Ň	ILE A	170	-7.1 7 5	34.395	14.463 14.562	1.00 1.00	64.35 76.83
	2898	CA	ILE A	170	-7.889	33.797	15.690	1.00	76.83
35	2899	CB	ILE A	170	-7.898	32.250	15.590	1.00	133.66
	2900	CG2	ILE A	170	-8.437	31.821	14.237	1.00	133.66
	2901 2902	CG1	ILE A	170	-6.482	31.697	15.761	1.00	133.66
	2902	CD1 C	ILE A	170 170	-6.386 7.106	30.180	15.647	1.00	133.66
40	2904	ŏ	ILE A	170	-7.196 -6.164	34.228 34.887	16.976 16.922	1.00 1.00	76.83 76.83
	2905	Ň	LYS A	171	-7.757	33.870	18.127	1.00	125.94
	2906	CA	LYS A	171	-7.152	34.252	19.397	1.00	125.94
	2907	CB	LYS A	171	-8.004	35.328	20.069	1.00	198.00
45	2908 2909	CD	LYS A LYS A	171	-9.449	34.922	20.293	1.00	198.00
73	2910	CE	LYS A	171 171	-10.354 -9.952	36.141 37.059	20.399	1.00	198.00
	2911	NZ.	LYS A	171	-10.825	38.268	21.546 21.607	1.00 1.00	198.00 198.00
	2912	С	LYS A	171	-6.957	33.072	20.338	1.00	125.94
5 0	2913	o	LYS A	171	-6.326	33.204	21.388	1.00	125.94
50	2914	<u>C1</u>	NAG A	221	13.561	29.146	-11.328	1.00	244.51
	2915 2916	C2 N2	NAG A	221	13.758	30.631	-11.596	1.00	244.51
	2917	C7	NAG A NAG A	221 221	12.475 12.407	31.303	-11.575	1.00	244.51
	2918	07	NAG A	221	13.396	32.594 33.270	-11.273 -10.988	1.00 1.00	244.51
55	2919	C8	NAG A	221	ر ۱۱.۵ د	33.233	-11.281	1.00	244.51 244.51
	2920	C3	NAG A	221	14.405	30.847	-12.952	1.00	244.51
	2921	03	NAG A	221	14.740	32.219	-13.099	1.00	244.51
	2922	C4	NAG A	221	15.661	29.997	-13.135	1.00	244.51
60	2923 2924	O4 C5	NAG A NAG A	221 221	16.044	30.091	-14.520	1.00	244.51
•	2925	O5	NAG A	221	15.375 14.809	28.530 28.456	-12.759 -11.436	1.00 1.00	244.51
	2926	C6	NAG A	221	16.622	27.665	-12.740	1.00	244.51 244.51
	2927	O 6	NAG A	221	17.566	28.140	-11.790	1.00	244.51
4 5	2928	C1	NAG A	222	17.330	29.723	-14.890	1.00	195.02
65	2929	C2	NAG A	222	17.910	30.770	-15.864	1.00	195.02
	2930 2931	N2 C7	NAG A	222	17.966	32.078	-15.229	1.00	195.02
	2932	07 ·	NAG A NAG A	222 222	19.134 20.210	32.692 32.206	-15.052	1.00	195.02
	2933	C8	NAG A	222	19.106	34.055	-15.404 -14.383	1.00 1.00	195.02 195.02
70	2934	C3	NAG A	222	17.061	30.835	-17.148	1.00	195.02

	2025	00	NAG 4		4= 45.4				
	2935 2936	03 C4	NAG A		17.694	31.675	-18.105	1.00	195.02
	2937	⊙ 4.	NAG A		16.869 15.938	29.431 29.494	-17.744	1.00	195.02
	2938	C5	NAG A		16.356	28.454	-18.814 -16.676	1.00	195.02
5	2939	O5	NAG A		17.249	28.441	-15.538	1.00 1.00	195.02
	2940	C6	NAG A		16.248	27.029	-17.174	1.00	195.02
	2941	O 6	NAG A		15.013	26.448	-16.789	1.00	195.02 195.02
	2942	C1	NAG A	242	-3.473	17.670	-6.472	1.00	81.55
10	2943	C2	NAG A	242	-3.080	17.582	-7.921	1.00	81.55
10	2944	N2	NAG A		-1.712	17.148	-8.025	1.00	81.55
	2945	C7	NAG A		-1.420	16.075	-8.748	1.00	81.55
	2946 2947	O7	NAG A		-2.270	15.414	-9.324	1.00	81.55
	2947 2948	C8 C3	NAG A		0.033	15.657	-8.846	1.00	81.55
15	2949	03	NAG A		-3.225 -2.918	18.933 18.814	-8.583	1.00	81.55
	2950	C4	NAG A		-4.642	19.456	-9.969 -8.403	1.00 1.00	81.55
	2951	04	NAG A		-4.712	20.825	-8.846	1.00	81.55
	2952	C5	NAG A		-5.062	19.392	-6.945	1.00	81.55 81.55
	2953	O5	NAG A		-4.830	18.086	-6.394	1.00	81.55
20	2954	C6	NAG A	242	-6.547	19.630	-6.824	1.00	81.55
	2955	O 6	NAG A		-6.826	20.697	-5. 933	1.00	81.55
	2956	C1	NAG A		-5.536	21.071	-9.934	1.00	123.88
	2957 2958	C2 N2	NAG A		-6.020	22.528	-9.929	1.00	123.88
25	2956 2959	N2 C7	NAG A		-6.814	22.800	-8.743	1.00	123.88
43	2960	O7	NAG A		-6.607 -5.746	23.908	-8.041	1.00	123.88
	2961	C8	NAG A		-7.482	24.727 24.135	-8.337 -6.820	1.00 1.00	123.88
	2962	C3	NAG A		-6.875	22.766	-11.173	1.00	123.88 123.88
	2963	O3	NAG A		-7.276	24.126	-11.231	1.00	123.88
30	2964	C4	NAG A	243	-6.109	22.379	-12.449	1.00	123.88
	2965	O4	NAG A		-7.002	22.470	-13.597	1.00	123.88
	2966	C5	NAG A		-5.608	20.937	-12.312	1.00	123.88
	2967	O5	NAG A		-4.793	20.809	-11.132	1.00	123.88
35	2968 2969	C6 O6	NAG A		-4.789	20.444	-13.485	1.00	123.88
33	2970	C1	MAN A	243 244	-3.560 -6.640	21.141 23.134	-13.577	1.00	123.88
	2971	C2	MAN A	244	-6.289	24. 639	-14.739 -14.645	1.00 1.00	177.21
	2972	02	MAN A	244	-4.892	24.794	-14.586	1.00	177.21 177.21
	2973	C3	MAN A	244	-6.845	25.182	-15.998	1.00	177,21
40	2974	O 3	MAN A	244	-6.636	26.575	-16.149	1.00	177.21
	2975	C4	MAN A	244	-6.314	24.396	-17.244	1.00	177.21
	2976	04	MAN A	244	-6.840	24.954	-18.451	1.00	177.21
	2977 2978	C5 O5	MAN A	244	-6.779	22.928	-17.096	1.00	177.21
45	2979	C6	MAN A	244 244	-6.232	22.337	-15.891	1.00	177.21
	2980	06	MAN A	244	-6.487 -5.159	22.037 21.562	-18.309	1.00	177.21
	2981	Č1	NAG A	250	18.849	18.682	-18.301 -1.016	1.00 1.00	177.21 245.89
	2982	C2	NAG A	250	19.989	19.613	-0.566	1.00	245.89 245.89
~~	2983	N2	NAG A	250	20.115	19.601	0.880	1.00	245.89
50	2984	C7	NAG A	250	21.178	19.048	1.458	1.00	245.89
	2985	07	NAG A	250	22.091	18.518	0.819	1.00	245.89
	2986	C8	NAG A	250	21.237	19.081	2.980	1.00	245.89
	2987 2988	င္သ	NAG A	250	19.696	21.039	-1.050	1.00	245.89
55	2989	03 C4	NAG A NAG A		20.782	21.896	-0.728	1.00	245.89
	2990	· 04	NAG A		19.457 19.058	21.047 22.347	-2.564 -2.977	1.00	245.89
	2991	C5	NAG A		18.367	20.028	-2.935	1.00 1.00	245.89
	2992	O5	NAG A		18.721	18.715	-2.444	1.00	245.89 245.89
	2993	C6	NAG A		18.165	19.903	-4.436	1.00	245.89
60	2994	O6	NAG A	250	17.400	18.748	-4.760	1.00	245.89
	2995	C1	NAG A		2.176	9.666	16.692	1.00	235.37
	2996	C2	NAG A		1.514	10.512	17.789	1.00	235.37
	2997 2998	N2 C7	NAG A		2.519	11.269	18.514	1.00	235.37
65	2999	C7 O7	NAG A NAG A		2.186	12.397	19.137	1.00	235.37
4	3000	C8	NAG A		1.042 3.289	12.855	19.128	1.00	235.37
	3001	ä	NAG A		0.750	13,134 9,604	19.882 18.761	1.00	235.37
	3002	03	NAG A		0.023	10.398	19.687	1.00 1.00	235.37 235.37
	3003	C4	NAG A		-0.216	8.687	18.005	1.00	235.37
70	3004	O4	NAG A		-0.794	7.758	18.909	1.00	235.37

	3005 3006	C5 O5	NAG NAG		0.534 1.187	7.934 8.871	16.900 16.018	1.00 1.00	235.37 235.37
	3007	C6	NAG .	A 274	-0.384	7.085	16.044	1.00	235.37
_	3008	O 6	NAG .	A 274	0.294	6.598	14.895	1.00	235.37
5	3009	C1	NAG	A 335	7.685	42.617	-1.591	1.00	248.30
	3010	C2	NAG	A 335	8.870	42.060	-0.765	1.00	248.30
	3011	N2	NAG .		8.767	42.587	0.583	1.00	248.30
	3012	C7	NAG .	A 335	8.573	41.777	1.618	1.00	248.30
	3013	O 7	NAG .		8.483	40.553	1.511	1.00	248.30
10	3014	C8	NAG .		8.472	42.430	2.987	1.00	248.30
	3015	C3	NAG		10.258	42.417	-1.325	1.00	248.30
	3016	Q3	NAG .		11.229	41.541	-0.771	1.00	248.30
	3017	C4	NAG		10.290	42.300	-2.841	1.00	248.30
15	3018	04	NAG .		11.560	42.706	-3.329	1.00	248.30
15	3019	C5	NAG		9.195	43.189	-3.414	1.00	248.30
	3020	O5	NAG		7.904	42.673	-3.021	1.00	248.30
	3021	C6	NAG A		9.222	43.210	-4.935	1.00	248.30
	3022 3023	O6	NAG A		9.423	44.524	-5.434	1.00	248.30
20	3023	C1 C2	NAG A		0.521	43.731	20.574	1.00	249.48
20	3025	N2	NAG A		-0.261	42.929	21.588	1.00	249,48
	3026	C7	NAG A		-1.284 -1.377	42.144	20.930	1.00	249.48
	3027	07 07	NAG		-0.627	40.843 40.266	21.191	1.00	249.48
	3028	C8	NAG A		-2.460	40.060	21.988 20.472	1.00	249.48
25	3029	C3	NAG		-0.877	43.866	22.605	1.00 1.00	249.48
	3030	03	NAG		-1.567	43.103	23.596	1.00	249.48 249.48
	3031	C4	NAG		0.234	44.689	23.266	1.00	249.48
	3032	04	NAG		-0.370	45.703	24.068	1.00	249.48
	3033	C 5	NAG /	A 340	1.188	45.334	22.220	1.00	249.48
30	3034	O 5	NAG /	A 340	1.601	44.382	21.233	1.00	249.48
	3035	C6	NAG A		2.460	45.780	22.881	1.00	249.48
	3036	O 6	NAG /		3.548	45.816	21.985	1.00	249.48
	3037	C1	NAG /		-14.447	34.952	2.337	1.00	170.79
35	3038	C2	NAG /		-15.009	34.055	1.250	1.00	170.79
55	3039 3040	N2 C7	NAG /		-14.171	34.149	0.073	1.00	170.79
	3040	07 07	NAG /		-13.171	33.289	-0.105	1.00	170.79
	3042	C8	NAG /		-12.912 -12.329	32.383 33.454	0.691 -1.361	1.00	170.79
	3043	ČŠ	NAG /		-16.425	34.482	0.910	1.00 1.00	170.79
40	3044	03	NAG A		-16.997	33.542	0.014	1.00	170.79 170.79
	3045	C4	NAG /		-17.290	34.565	2.168	1.00	170.79
	3046	04	NAG /	A 366	-18.549	35.187	1.824	1.00	170,79
	3047	C5	NAG A	A 366	-16.584	35.380	3.275	1.00	170.79
4.5	3048	Q 5	NAG /		-15.258	34.873	3.503	1.00	170.79
45	3049	C6	NAG /		-17.297	35.315	4.613	1.00	170.79
	3050	0 6	NAG /		-16.620	36.092	5.592	1.00	170.79
	3051	C1	NAG /		-19.711	34.493	2.163	1.00	247.02
	3052 3053	C2 N2	NAG /		-20.892	35.462	2.268	1.00	247.02
50	3054	C7	NAG /		-20.619	36.488	3.255	1.00	247.02
50	3055	07 07	NAG /		-20.363 -20.347	37.730	2.856	1.00	247.02
	3056	C8	NAG /		-20.347	38.061 38.762	1.668	1.00	247.02
	3057	ä	NAG A		-22.151	34.676	3.937	1.00	247.02
	3058	03	NAG A		-23.265	35.554	2.640 2.696	1.00 1.00	247.02
55	3059	C4	NAG /		-22.395	33.586	1.591	1.00	247.02 247.02
	3060	04	NAG A		-23 511	32.793	1.970	1.00	247.02
	3061	C5	NAG /	367	-21.148	32.698	1.448	1.00	247.02
	3062	O 5	NAG A	367	-19.981	33.508	1.147	1.00	247.02
<i>c</i> 0	3063	C6	NAG /		-21.291	31.682	0.332	1.00	247.02
60	3064	06	NAG A		-20.416	31.974	-0.749	1.00	247.02
	3065	CB	LYS E		28.538	57.342	22.861	1.00	248.35
	3066	CG CD	LYS E		28.723	58.799	22.474	1.00	248.35
	3067 3068	CD	LYS		28.723	59.692	23.702	1.00	248.35
65	3069	CE NZ	LYS E		28.914	61.151	23.330	1.00	248.35
55	3070	C	LYS E		28.914 29.934	62.022	24.537	1.00	248.35
	3071	ŏ	LYS E		29.93 4 30.913	56.599 57.081	20.941	1.00	249.33
	3072	Ň	LYS		28.491	57.081 54.970	21.514 22.165	1.00	249.33
	3073	CA	LYS		28.619	56.377	22.165 21. 68 3	1.00 1.00	249.33 249.33
70	3074	N	PRO E		29.974	56.244	19.648	1.00	115.49
									. 10.73

	3075	CD	PRO B	5 -	28.994	55.392	18.958	1.00	70.51
	3076 3077	CA CB	PRO B	5	31.186	56.414	18.835	1.00	115.49
	3078	CG	PRO B	5	31.037	55.337	17.765	1.00	70.51
5	3079	C	PRO B	5 5	29.573 31.329	55.299 57.007	17.553	1.00	70.51
	3080	ŏ	PRO B	5	30.350	57.807 58.537	18.247	1.00	115.49
	3081	Ň	LYS B	6	32.553	58.174	18.126 17.885	1.00	115.49
	3082	CA	LYS B	6	32.811	59.492	17.331	1.00 1.00	105.72
	3083	СВ	LYS B	6	33.258	60.458	18.449	1.00	105.72
10	3084	CG	LYS B	6	33.432	61.901	17.991	1.00	206.94 206.94
	3085	CD	LYS B	6	33.697	62.850	19.152	1.00	206.94
	3086	CE	LYS B	6	33.826	64.287	18.654	1.00	206.94
	3087	NZ	LYS B	6	34.006	65.275	19.759	1.00	206.94
15	3088	C	LYS B	6	33.857	59.42 9	16.222	1.00	105.72
13	3089	0	LYS B	6	35.018	59.109	16.467	1.00	105.72
	3090 3091	N CA	VAL B	7	33.433	59.742	15.002	1.00	68.17
	3092	CB	VAL B	7	34.317	59.728	13.843	1.00	68.17
	3093	CG1	VAL B	7 7	33.553 34.487	59.960 50.738	12.545	1.00	86.47
20	3094	CG2	VAL B	7	32.346	59.738 59.072	11.359 12.479	1.00	86.47
	3095	Č	VAL B	7	35.401	60.796	13.845	1.00 1.00	86.47
	3096	Ō	VAL B	7	35.094	61.988	13.803	1.00	68.17
	3097	N	SER B	8	36.661	60.385	13.864	1.00	68.17 61.68
~-	3098	CA	SER B	8	37.741	61.355	13.837	1.00	61.68
25	3099	CB	SER B	8	38.836	60.969	14.842	1.00	135.50
	3100	OG	SER B	8	39.289	59.647	14.622	1.00	135.50
	3101	C	SER B	8	38.303	61.405	12.406	1.00	61.68
	3102	0	SER B	8	38.019	60.525	11.594	1.00	61.68
30	3103	N CA	LEU B	9	39.092	62.435	12.106	1.00	91.60
50	3104 3105	CA CB	LEU B	9	39.699	62.594	10.790	1.00	91.60
	3106	CG	LEU B	9	39.080	63.779	10.053	1.00	67.13
	3107	CD1	LEU B	9 9	37.601 37.378	63.806 64.735	9.688	1.00	67.13
	3108	CD2	LEU B	9	37.167	62.435	8.524 9.291	1.00	67.13
35	3109	C	LEU B	9	41.195	62.847	10.897	1.00 1.00	67.13
	3110	0	LEU B	9	41.675	63.347	11.915	1.00	91.60 91.60
	3111	N	ASN B	10	41.928	62.519	9.835	1.00	84.59
	3112	CA	ASN B	10	43.369	62.742	9.800	1.00	84.59
40	3113	CB	ASN B	10	44.107	61. 64 0	10.548	1.00	140.61
40	3114	CG	ASN B	10	45.558	61. 97 8	10.763	1.00	140.61
	3115	OD1	ASN B	10	45.889	62.905	11.505	1.00	140.61
	3116 3117	ND2 C	ASN B	10	46.438	61.241	10.099	1.00	140.61
	3118	ŏ	ASN B	10 10	43.876	62.812	8.367	1.00	84.59
45	3119	Ň	PRO B	11	43.883 44.310	61.805 64.010	7.656	1.00	84.59
	3120	CD	PRO B	11	44.699	64.185	7.917 6.506	1.00	77.61
	3121	CA	PRO B	11	44.370	65.289	8.638	1.00 1.00	115.85
	3122	CB	PRO B	11	44.811	66.264	7.544	1.00	77.61 115.85
~~	3123	CG	PRO B	11	45.560	65.394	6.570	1.00	115.85
50	3124	С	PRO B	11	43.042	65.731	9.290	1.00	77,61
	3125	0	PRO B	11	41.982	65.231	8.937	1.00	77.61
	3126	N	PRO B	12	43.085	66.680	10.239	1.00	88.06
	3127	CD	PRO B	12	44.279	67.378	10.753	1.00	174.82
55	3128	CA CB	PRO B	12	41.883	67.170	10.921	1.00	88.06
55	3129 3130	CB CG	PRO R	12	42.433	68.119	11.982	1.00	174.82
	3131	C	PRO B	12	43.854	67.699	12.148	1.00	174.82
	3132	ŏ	PRO B	12 12	40.993 39.781	67.939 68.071	9.924	1.00	88.06
	3133	Ň	TRP B	13	41.623	68.071 68.464	10.108 8.880	1.00	88.06
60	3134	CA	TRP B	13	40.932	69.239	7.859	1.00 1.00	96.43 96.43
	3135	СВ	TRP B	13	41.907	69.605	6.731	1.00	96.43 96.49
	3136	CG	TRP B	13	43.190	70.134	7.232	1.00	96.49
	3137	CD2	TRP B	13	43.376	70.974	8.358	1.00	96.49
65	3138	CE2	TRP B	13	44.757	71.168	8.509	1.00	96.49
65	3139	CE3	TRP B	13	42.504	71.588	9.268	1.00	96.49
	3140	CD1	TRP 8	13	44.423	69.863	6.745	1.00	96.49
	3141 3142	NE1 CZ2	TRP B	13	45.373	70.474	7.506	1.00	96.49
	3143	CZ3	TRP B	13 13	45.298	71.947	9.532	1.00	96.49
70	3144	CH2	TRP B	13	43.034 44.424	72.363 72.536	10.283	1.00	96.49
	•	~· · · · ·	5	13	TT.764	72.536	10.410	1.00	96.49

	3145 3146	C	TRP B	13 13	39.742 39.882	68.497 67.403	7.281 6.738	1.00	96.43
	3147	N	ASN B	14	38.567	69.102	7.407	1.00 1.00	96.43
_	3148	CA	ASN B	14	37.352	68.509	6.867	1.00	72.14
5	3149	CB	ASN B	14	36.239	68.455	7.931	1.00	72.14 117.87
	3150	CG	ASN B	14	35.712	69.812	8.309	1.00	117.87
	3151 3152	OD1 ND2	ASN B	14	36.462	70.695	8.718	1.00	117.87
	3153	C	ASN B ASN B	14 14	34.407	69.984	8.184	1.00	117.87
10	3154	ŏ	ASN B	14	36.858 35.721	69.201 69.018	5.588 5.177	1.00	72.14
	3155	Ň	ARG B	15	37.715	70.009	4.973	1.00 1.00	72.14
	3156	CA	ARG B	15	37.399	70.653	3.701	1.00	61.00 61.00
	3157	CB	ARG B	15	37.241	72.149	3.841	1.00	68.74
15	3158	CG	ARG B	15	36.513	72.569	5.064	1.00	68.74
13	3159 3160	CD NE	ARG B	15	36.354	74.075	5.045	1.00	68.74
	3161	CZ	ARG B ARG B	15 15	35.436	74.525	4.007	1.00	68.74
	3162	NH1	ARG B	15 15	35.531 36.501	75.714 76.533	3.429	1.00	68.74
	3163	NH2	ARG B	15	34.660	76.093	3.794 2.498	1.00 1.00	68.74
20	3164	С	ARG B	15	38.662	70.393	2.900	1.00	68.74 61.00
	3165	0	ARG B	15	39.707	70.950	3.199	1.00	61.00
	3166	N	ILE B	16	38.587	69.540	1.895	1.00	73.69
	3167 3168	CA CB	ILE B	16	39.770	69.256	1.135	1.00	73.69
25	3169	CG2	ILE B	16 16	40.194	67.833	1.339	1.00	63.86
	3170	CG1	ILE B	16	40.624 39.044	67.645 66.895	2.767	1.00	63.86
	3171	CD1	ILE B	16	39.388	65.448	0. 994 1.178	1.00 1.00	63.86
	3172	С	ILE B	16	39.621	69.493	-0.340	1.00	63.86 73.69
20	3173	0	ILE B	16	38.516	69.651	-0.866	1.00	73.69
30	3174	N	PHE B	17	40.770	69.491	-0.998	1.00	99.56
	3175 3176	CA CB	PHE B PHE B	17	40.889	69.696	-2.425	1.00	99.56
	3177	CG	PHE B PHE B	17 17	42.282 42.400	70.211	-2.720	1.00	81.03
	3178	CD1	PHE B	17	43.515	71.703 72.315	-2.699 -2.128	1.00 1.00	81.03
35	3179	CD2	PHE B	17	41.453	72.497	-3.344	1.00	81.03 81.03
	3180	CE1	PHE B	17	43.685	73.688	-2.204	1.00	81.03
	3181	CE2	PHE B	17	41.613	73.877	-3.428	1.00	81.03
	3182 3183	cz	PHE B	17	42.733	74.475	-2.860	1.00	81.03
40	3184	C	PHE B PHE B	17 17	40.678	68.392	-3.169	1.00	99.56
	3185	Ň	LYS B	18	40.804 40.374	67.321 68.484	-2.591	1.00	99.56
	3186	CA	LYS B	18	40.160	67.302	-4.459 -5.288	1.00 1.00	100.47
	3187	CB	LYS B	18	39.700	67.733	-6.682	1.00	100.47 201.96
45	3188	CG	LYS B	18	39.302	66.601	-7.612	1.00	201.96
43	3189	CD	LYS B	18	38.552	67.166	-8.809	1.00	201.96
	3190 3191	CE NZ	LYS B LYS B	18	38.122	66.086	-9.776	1.00	201.96
	3192	C	LYS B	18 18	39.299 41.448	65.382 66.402	-10.345	1.00	201.96
	3193	ŏ	LYS B	18	42.518	66.492 67.028	-5.394 -5.671	1.00	100.47
50	3194	N	GLY B	19	41.362	65.197	-5.143	1.00 1.00	100.47 85.25
	3195	CA	GLY B	19	42.547	64.371	-5.264	1.00	85.25
	3196	C	GLY B	19	43.350	64.115	-4.008	1.00	85.25
	3197 3198	O	GLY B	19	44.237	63.274	-3.996	1.00	85.25
55	3199	N CA	GLU B GLU B	20 20	43.057	64.825	-2.937	1.00	70.09
	3200	CB	GLU B	20	43.804 43.005	64.606 65.846	-1.701	1.00	70.09
	3201	ČĞ	GLU B	20	44.020	67.133	-0.813 -1.566	1.00	167.13
	3202	CD	GLU B	20	44.034	68.357	-0.677	1.00 1.00	167.13 167.13
60	3203	OE1	GLU B	20	43.009	68.622	-0.013	1.00	167.13
60	3204	OE2	GLU B	20	45.070	69.056	-0.655	1.00	167.13
	3205 3206	C	GLU B	20	43.296	63.356	-0.967	1.00	70.09
	3207	0 N	GLU B ASN B	20	42.273	62.769	-1.368	1.00	70.09
	3208	CA	ASN B	21 21	44.002 43.579	62.935 61.747	0.086	1.00	77.36
65	3209	CB	ASN B	21	44.626	60.630	0.830 0.8 0 2	1.00	77.36
	3210	CG	ASN B	21	45.285	60.472	-0.537	1.00 1.00	155.50 155.50
	3211	OD1	ASN B	21	44.634	60.520	-1.585	1.00	155.50
	3212	ND2	ASN B	21	46.598	60.265	-0.490	1.00	155.50
70	3213 3214	C	ASN B ASN B	21	43.300	62.066	2.287	1.00	77.36
. •		9	7014 B	21	43.997	62.877	2.892	1.00	77.36

	3215	N	VAL B	22	42.286	61.409	2.848	1.00	•••
	3216	CA	VAL B	22	41.899	61.602	4.241	1.00 1.00	68.07
	3217	CB	VAL B	22	40.732	62.572	4.364	1.00	68.07 74.66
5	3218	CG1	VAL B	22	39.514	62.023	3.658	1.00	74.66
,	3219 3220	CG2 C	VAL B	22	40.438	62.807	5.811	1.00	74.66
	3221	ŏ	VAL B VAL B	22 22	41.469	60.270	4.829	1.00	68.07
	3222	Ň	THR B	23	40.964 41.646	59.391 60.123	4.120	1.00	68.07
	3223	CA	THR B	23	41.316	58.865	6.1 32 6.791	1.00 1.00	73.02
10	3224	CB	THR B	23	42.576	58.274	7.428	1.00	73.02 107.36
	3225	OG1	THR B	23	43.602	58.155	6.435	1.00	107.36
	3226 3227	CG2	THR B	23	42.288	56.919	8.018	1.00	107.36
	3228	C O	THR B THR B	23	40.278	59.057	7.885	1.00	73.02
15	3229	Ň	LEU B	23 24	40.446 39.211	59.918	8.739	1.00	73.02
	3230	CA	LEU B	24	38.180	58.261 58.423	7.888 8.920	1.00	82.14
	3231	СВ	LEU B	24	36.771	58.497	8.323	1.00 1.00	82.14
	3232	CG	LEU B	24	36.534	59.233	6.996	1.00	67.63 67.63
20	3233	CD1	LEU B	24	35.063	59.448	6.787	1.00	67.63
20	3234 3235	CD2 C	LEU B LEU B	24	37.249	60.554	6.987	1.00	67.63
	3236	ŏ	LEU B LEU B	24 24	38.205	57.286	9.904	1.00	82.14
	3237	Ň	THR B	25	37. 73 2 38.735	56.195 57.551	9.615	1.00	82.14
	3238	CA	THR B	25	38.817	56.519	11.086 12.099	1.00 1.00	78.19
25	3239	СВ	THR B	25	2.047	56.755	12.971	1.00	78.19 154.05
	3240	OG1	THR B	25	41.200	56.846	12.124	1.00	154.05
	3241 3242	CG2	THR B	25	40.231	55.618	13.949	1.00	154.05
	3243	C O	THR B THR B	25 25	37.554	56.489	12.941	1.00	78.19
30	3244	Ň	CYS B	25 26	37.022 37.044	57.532 55.296	13.310	1.00	78.19
	3245	CA	CYS B	26	35.860	55.184	13.210 14.049	1.00 1.00	82.94
	3246	С	CYS B	26	36.280	55.187	15.510	1.00	82.94 82.94
	3247	0	CYS B	26	37.254	54.549	15.896	1.00	82.94
35	3248 3249	CB	CYS B	26	35.094	53.908	13.763	1.00	125.46
JJ	3250	SG N	CYS B ASN B	26 27	33.481	53.869	14.604	1.00	125.46
	3251	CA	ASN B	27 27	35 .53 5 35.784	55.931	18.309	1.00	247.26
	3252	CB	ASN B	27	34.500	56.058 55.740	17.730 18.470	1.00 1.00	247.26
40	3253	CG	ASN B	27	34.506	56.280	19.864	1.00	240.69 240.69
40	3254	OD1	ASN B	27	35.033	57.371	20.107	1.00	240.69
	3255 3256	ND2	ASN B	27	33.909	55.541	20.797	1.00	240.69
	3257	C	ASN B ASN B	27	36.922	55.201	18.289	1.00	247.26
	3258	Ň	GLY B	27 28	36.702 38.135	54.072 55.748	18.722	1.00	247.26
45	3259	CA	GLY B	28	39.286	55.021	18.286 18.792	1.00 1.00	195.90
	3260	C	GLY B	28	40.518	55.841	18.506	1.00	195.90 195.90
	3261	. 0	GLY B	28	40.788	56.161	17.355	1.00	195.90
	3262 3263	N CA	ASN B	29	41.274	56.181	19.541	1.00	230.48
50	3264	CB	ASN B ASN B	29 29	42.456	57.003	19.352	1.00	230.48
	3265	CG	ASN B	29	42.882 43.919	57.612 58.710	20.690	1.00	249.51
	3266	OD1	ASN B	29	44.154	59.198	20.527 19.421	1.00 1.00	249.51
	3267	ND2	ASN B	29	44.534	59.115	21.634	1.00	249.51 249.51
55	3268	C	ASN B	29	43.644	56.302	18.699	1.00	230.48
33	3269 3270	0 N	ASN B	29	44.198	56.804	17.716	1.00	230.48
	3271	CA	ASN B ASN B	30 30	44.040	55.149	19.229	1.00	218.47
	3272	CB	ASN B	30	45.185 46.364	54.441 54.509	18.667	1.00	218.47
	3273	CG	ASN B	30	46.841	55.909	19.631 19.854	1.00 1.00	238.45 238.45
60	3274	OD1	ASN B	30	46.936	56.337	20.986	1.00	238.45
	3275	ND2	ASN B	30	47.139	56.635	18.778	1.00	238.45
	3276 3277	C	ASN B	30	44.936	52.990	18.293	1.00	218.47
	3278	N	ASN B PHE B	30	44.881	52.646	17.109	1.00	218.47
65	3279	ČA	PHE B	31 31	44.779 44.573	52.137 50.734	19.300	1.00	249.37
	3280	CB	PHE B	31	44.573 45.620	50.724 49.901	19.037 19. 79 9	1.00	249.37
	3281	CG	PHE B	31	47.045	50.311	19.513	1.00 1.00	234.42 234.42
	3282	CD1	PHE B	31	47.600	51.429	20.131	1.00	234.42 234.42
70	3283 3284	CD2 CE1	PHE B	31	47.822	49.594	18.607	1.00	234.42
, ,	JEUH	GET	PHE B	31	48.909	51.828	19.854	1.00	234.42

	3285	CE2	PHE B	31-	49.131	49.985	18.322	1.00	234.42
	3286	cz	PHE B	31	49.674	51.107	18. 947	1.00	234.42
	3287 3288	C	PHE B	31	43.166	50.221	19.340	1.00	249.37
5	3289	0 N	PHE B PHE B	31	42.638	50.399	20.440	1.00	249.37
,	3290	CA CA	PHE B	32 32	42.579	49.581	18.332	1.00	162.47
	3291	CB	PHE B	32	41.233 40.337	49.034 49.732	18.408	1.00	162.47
	3292	CG	PHE B	32	38.872	49.480	17.386 17.598	1.00	249.69
	3293	CD1	PHE B	32	38.241	49.969	18.718	1.00 1.00	249.69
10	3294	CD2	PHE B	32	38.130	48.733	16.690	1.00	249.69
	3295	CE1	PHE B	32	36.894	49.721	18.931	1.00	249.69
	3296	CE2	PHE B	32	36.772	48.482	16.901	1.00	249.69 249.69
	3297	CZ	PHE B	32	36.170	48.988	18.039	1.00	249.69
16	3298	Ç	PHE B	32	41.243	47.533	18.118	1.00	162.47
15	3299	0	PHE B	32	42.275	46.987	17.714	1.00	162.47
	3300	N	GLU B	33	40.097	46.869	18.298	1.00	249.28
	3301 3302	CA CB	GLU B	33	40.035	45.425	18.046	1.00	249.28
	3303	CG	GLU B GLU B	33	39.767	44.643	19.298	1.00	249.25
20	3304	CD	GLU B	33 33	39.978	43.139	19.158	1.00	249.25
	3305	OE1	GLU B	33	41.395 42.373	42.776 43.401	18.727	1.00	249.25
	3306	OE2	GLU B	33	41.565	41.829	19.192 17.938	1.00	249.25
	3307	c	GLU B	33	38.993	44.918	17.083	1.00 1.00	249.25
	3308	0	GLU B	33	39.312	44.164	16.171	1.00	249.28 249.28
25	3309	N	VAL B	34	37.732	45.243	17.348	1.00	234.23
	3310	CA	VAL B	34	36.657	44.756	16.507	1.00	234.23
	3311	CB	VAL B	34	35.301	45.388	16.902	1.00	191.69
	3312	CG1	VAL B	34	34.197	44.865	15.998	1.00	191.69
30	3313	CG2	VAL B	34	34.978	45.059	18.343	1.00	191.69
50	3314 3315	C O	VAL B	34	36.919	44.972	15.029	1.00	234.23
	3316	Ň	VAL B SER B	34	37.592	45.923	14.632	1.00	234.23
	3317	GA	SER B	35 35	36.395 36.536	44.052 44.110	14.229	1.00	249.39
	3318	CB	SER B	35	37.053	44.110 42.775	12.789	1.00	249.39
35	3319	ÖĞ	SER B	35	36.078	41.759	12.246 12.404	1.00 1.00	187.29
	3320	C	SER B	35	35.161	44.414	12.202	1.00	187.29 249.39
	3321	0	SER B	35	35.008	44.523	10.988	1.00	249.39
	3322	N	SER B	36	34.160	44.541	13.074	1.00	236.03
40	3323	CA	SER B	36	32.796	44.846	12.641	1.00	236.03
40	3324	CB	SER B	36	31.770	43.967	13.369	1.00	174.69
	3325	og	SER B	36	31.663	44.323	14.735	1.00	174.69
	3326 3327	C	SER B	36	32.488	46.310	12.911	1.00	236.03
	3328	0 N	SER B THR B	36 37	32.037	46.684	13.992	1.00	236.03
45	3329	CA	THR B	37	32.752 32.516	47.137 48.565	11.910	1.00	186.56
	3330	CB	THR B	37	33.852	49.349	11.996 11.926	1.00 1.00	186.56
	3331	OG1	THR B	37	34.720	48.919	12.983	1.00	204.69
	3332	CG2	THR B	37	33.611	50.838	12.065	1.00	204.69 204.69
~~	3333	С	THR B	37	31.649	48.899	10.789	1.00	186.56
50	3334	0	THR B	37	31.837	A8.338	9.708	1.00	186.56
	3335	N	LYS B	38	30.692	49.800	10.972	1.00	233.53
	3336	CA	LYS B	38	29.803	50.182	9.883	1.00	233.53
	3337	CB	LYS B	38	28.358	50.059	10.341	1.00	159.29
55	3338 3339	CG	LYS B	38	28.005	48.688	10.851	1.00	159.29
33	3340	CD CE	LYS B	38	26.556	48.633	11.299	1.00	159.29
	3341	NZ	LYS B LYS B	38 38	26.179 24.755	47.229 ·	11.738	1.00	159.29
	3342	Ċ	LYS B	38	24.755 30.055	47.156 51.604	12.158	1.00	159.29
	3343	ŏ	LYS B	38	30.349	52.490	9.402 10.203	1.00 1.00	233.53
60	3344	Ň	TRP B	39	29.936	51.818	8.092	1.00	233.53 87.42
	3345	CA	TRP B	39	30.140	53.149	7.521	1.00	87.42
	3346	CB	TRP B	39	31.422	53.229	6.688	1.00	107.80
	3347	CG	TRP B	39	32.678	53.035	7.471	1.00	107.80
45	3348	CD2	TRP B	39	33.240	53.923	8.438	1.00	107.80
65	3349	CE2	TRP B	39	34.427	53.326	8.904	1.00	107.80
	3350	CE3	TRP B	39	32.857	55.160	8.954	1.00	107.80
	3351 3352	CD1 NE1	TRP B	39	33.521	51.968	7.395	1.00	107.80
	3352 3353	CZ2	TRP B	39	34.574	52.135	8.253	1.00	107.80
70	3354	CZ3	TRP B	39 30	35.236	53.930 55.755	9.860	1.00	107.80
		س	IRF D	39	33.659	55.755	9.899	1.00	107.80

	3355 3356 3357	CH2 C O	TRP B TRP B TRP B	39 39 39	34.839 28.973 28.580	55.141 53.500 52.712	10.346 6.637	1.00 1.00	107.80 87.42
	3358	Ň	PHE B	40	28.429	54.694	5.79 9 6.818	1.00	87.42
5	3359	CA	PHE B	40	27.289	55,111	6.025	1.00 1.00	127.18
	3360	CB	PHE B	40	26.052	55.264	6.908	1.00	127.18 155.57
	3361	CG	PHE B	40	25.605	54.032	7.687	1.00	155.57
	3362	CD1	PHE B	40	26.374	53.715	8.858	1.00	155.57
10	3363 3364	CD2 CE1	PHE B	40	24.666	53.200	7.261	1.00	155.57
10	3365	CE2	PHE B PHE B	40 40	26.024	52.589 52.074	9.600	1.00	155.57
	3366	CZ	PHE B	40	24.308 24.987	52.074 51.764	7.991 9.162	1.00	155.57
	3367	Ċ.	PHE B	40	27.523	56.414	5.102 5.281	1.00 1.00	155.57 127.18
	3368	0	PHE B	40	27.208	57.495	5.773	1.00	127.18
15	3369	N	HIS B	41	28.078	56.306	4.084	1.00	72.05
	3370	CA	HIS B	41	28.329	57.484	3.260	1.00	72.05
	3371 3372	CB CG	HIS B HIS B	41	29.355	57.132	2.173	1.00	83.13
	3373	CD2	HIS B	41 41	29.650 29.801	58.256 58.274	1.230	1.00	83.13
20	3374	ND1	HIS B	41	29.837	59.553	-0.114 1.656	1.00 1.00	83.13
	3375	CE1	HIS B	41	30.087	60.323	0.614	1.00	83.13 83.13
	3376	NE2	HIS B	41	30.071	59.571	-0.472	1.00	83.13
	3377	C	HIS B	41	27.010	57.961	2.633	1.00	72.05
25	3378	0	HIS B	41	26.458	57.298	1.761	1.00	72.05
43	3379 3380	N CA	ASN B ASN B	42 42	26.527	59.123	3.069	1.00	104.44
	3381	CB	ASN B	42 42	25.256 25.240	59.683 59.870	2.600	1.00	104.44
	3382	ČĞ	ASN B	42	26.091	61.039	1.077 0. 62 5	1.00 1.00	64.53
	3383	OD1	ASN B	42	27.195	61.213	1.144	1.00	64.53 64.53
30	3384	ND2	ASN B	42	25.618	61.828	-0.348	1.00	64.53
	3385	C	ASN B	42	24.114	58.751	2.999	1.00	104.44
	3386 3387	O N	ASN B GLY B	42	23.089	58.706	2.334	1.00	104.44
	3388	CA	GLY B	43 43	24.293 23.246	58.003 57.092	4.083	1.00	163.92
35	3389	Č	GLY B	43	23.405	57.092 55. 67 7	4.522 3.991	1.00 1.00	163.92 163.92
	3390	0	GLY B	43	23.159	54.701	4.702	1.00	163.92
	3391	N	SER B	44	23.816	55.562	2.735	1.00	175.12
	3392	CA	SER B	44	24.017	54.262	2.106	1.00	175.12
40	3393 3394	CB OG	SER B	44	24.326	54.445	0.620	1.00	173.04
70	3395	C	SER B SER B	44 44	23.344 25.178	55.253 53.524	-0.002	1.00	173.04
	3396	ŏ	SER B	44	26.275	54.070	2.772 2.8 9 9	1.00 1.00	175.12
	3397	N	LEU B	45	24.944	52.285	3.197	1.00	175.12 151.43
15	3398	CA	LEU B	45	25.991	51.495	3.846	1.00	151.43
45	3399	CB	LEU B	45	25.458	50.101	4.198	1.00	163.91
	3400 3401	CG CD1	LEU B LEU B	45	26.424	49.160	4.922	1.00	163.91
	3402	CD2	LEU B	45 45	26.972 25.701	49.825	6.176	1.00	163.91
	3403	C	LEU B	45	27.220	47.872 51 .376	5.275 2.944	1.00 1.00	163.91
50	3404	0	LEU B	45	27.089	51.318	1.722	1.00	151.43 151.43
	3405	N	SER B	46	28.411	51.350	3.541	1.00	127.11
	3406	CA	SER B	46	29.646	51.241	2.770	1.00	127.11
	3407 3408	CB CC	SER B	46	30.724	52.142	3.366	1.00	226.86
55	3409	OG C	SER B SER B	46 46	31.902	52.103	2.574	1.00	226.86
	3410	ŏ	SER B	46	30.103 29.622	49.791 49.009	2.810 3.626	1.00	127.11
	3411	N	GLU B	47	31.030	49.425	1.927	1.00 1.00	127.11 149.05
	3412	CA	GLU B	47	31.486	48.041	1.929	1.00	149.05
60	3413	CB	GLU B	47	31.711	47.509	0.484	1.00	195.89
OU	3414	CG	GLU B	47	30.777	48.077	-0.608	1.00	195.89
	3415 3416	CD OE1	GLU B GLU B	47 47	31.343	47.934	-2.030	1.00	195.89
	3417	OE2	GLU B	47	32.086 31.042	48.832 46.909	-2.508 -2.695	1.00	195.89
	3418	Č	GLU B	47	32.738	47.807	-2.685 2.808	1.00 1.00	195.89
65	3419	0	GLU B	47	33.224	46.684	2.891	1.00	149.05 149.05
	3420	N	GLU B	48	33.291	48.851	3.436	1.00	101.79
	3421	CA	GLU B	48	34.458	48.628	4.299	1.00	101.79
	3422 3423	CB CG	GLU B	48	35.331	49.904	4.457	1.00	223,78
70	3424	CD	GLU B GLU B	48 48	36.479 37.584	49.790	5.499 5.107	1.00	223.78
		~ -	~CO D	70	Jr.J04	48.801	5.127	1.00	223.78

	3425	OE1	GLU B	48	38.340	49.074	4.170	1.00	000 70
	3426	OE2	GLU B	48	37.703	47.751	5.799		223.78
	3427	С	GLU B	48	33.949	48.158	5.661	1.00	223.78
_	3428	0	GLU B	48	32.788	48.397	6.021	1.00	101.79
5	3429	Ň	THR B	49	34.812	47.476		1.00	101.79
	3430	CA	THR B	49	34.445	46.976	6.410	1.00	169.38
	3431	СВ	THR B	49	34.268	45.441	7.728	1.00	169.38
	3432	OG1	THR B	49	35.467	-	7.707	1.00	162.45
	3433	CG2	THR B	49		44.824	7.222	1.00	162.45
10	3434	C	THR B	49	33.110	45.061	6.797	1.00	162,45
	3435	ŏ	THR B		35.501	47.369	8.762	1.00	169.38
	3436	Ň	ASN B	49	35.190	47.530	9.940	1.00	169.38
	3437	ČA		50	36.745	47.531	8.319	1.00	110.90
	3438		ASN B	50	37.830	47.919	9.213	1.00	110.90
15		CB	ASN B	50	39.130	48.104	8.418	1.00	249.40
13	3439	CG	ASN B	50	40.355	48.183	9.311	1.00	249.40
	3440	OD1	ASN B	50	40.232	48.440	10.508	1.00	249.40
	3441	ND2	ASN B	50	41.539	47.979	8.738	1.00	249.40
	3442	Č	ASN B	50	37.403	49.246	9.854	1.00	110,90
20	3443	0	ASN B	50	36.644	50.010	9.250	1.00	110.90
20	3444	N	SER B	51	37.872	49.520	11.072	1.00	116.16
	3445	CA	SER B	51	37.515	50.763	11.761	1.00	116.16
	3446	CB	SER B	51	38.004	50.728	13.210	1.00	
	3447	OG	SER B	51	39.421	50.782	13.277	1.00	152.88
	3443	С	SER B	51	38.084	52.007	11.066	1.00	152.88
25	3449	0	SER B	51	37.632	53.121	11.313		116.16
	3450	N	SER B	52	39.080	51.819		1.00	116.16
	3451	CA	SER B	52	39.684	52.939	10.206	1.00	154.44
	3452	СВ	SER B	52	41.210	52.899	9.501	1.00	154.44
	3453	ÖĞ	SER B	52	41.611		9.637	1.00	81.31
30	3454	Č	SER B	52	39.294	53.078	10.987	1.00	81.31
	3455	ŏ	SER B	52 52		52.908	8.036	1.00	154.44
	3456	Ň	LEU B		39.754	52.057	7.273	1.00	154.44
	3457	CA	LEU B	53	38.433	53.844	7.656	1.00	115.15
	3458	CB		53	37.961	53.963	6.280	1.00	115.15
35	3459	CG		53	36.477	54.348	6.281	1.00	65.06
55	3460		LEU B	53	35.882	55.021	5.036	1.00	65.06
		CD1	LEU B	53	36.353	54.301	3.774	1.00	65.06
	3461	CD2	LEU B	53	34.357	55.039	5.132	1.00	65.06
	3462	C	LEV B	53	38.775	55.005	5.509	1.00	115.15
40	3463	0	LEU B	53	38.547	56.20 9	5.659	1.00	115.15
40	3464	N	ASN B	54	39.712	54.549	4.676	1.00	78.33
	3465	CA	ASN B	54	40.533	55.488	3.918	1.00	78.33
	3466	CB	ASN B	54	41.826	54.832	3.460	1.00	116.91
	3467	ÇG	ASN B	54	42.792	54.609	4.598	1.00	116.91
4.5	3468	OD1	ASN B	54	43.166	55.545	5.307	1.00	116.91
45	3469	ND2	ASN B	54	43.204	53.364	4.782	1.00	116.91
	3470	С	ASN B	54	39.834	56.084	2.716	1.00	78.33
	3471	0	ASN B	54	38.853	55.548	2.226	1.00	78.33
	3472	N	ILE B	55	40.333	57.227	2.269	1.00	83.98
	3473	CA	ILE B	55	39.800	57.906	1.100	1.00	83.98
50	3474	CB	ILE B	55	38.973	59.141	1.493	1.00	67.63
	3475	CG2	ILE B	55	38.828	60.092	0.322	1.00	67.63
	3476	CG1	ILE B	55	37.598	58.686	1.980	1.00	
	3477	CD1	ILE B	55	36.675	59.826	2.438	4 4-	67.63
	3478	С	ILE B	55	41.015	58.329	0.298	1.00	67.63
55	3479	0	ILE B	55	41.882	59.043	0.805		83.98
	3480	N	√AL B	56	41.099	57.866		1.00	83.98
	3481	CA	VAL B	56	42.231	58.216	-0.942	1.00	110.45
	3482	CB	VAL B	56	42.737	56.993	-1.781	1.00	110.45
	3483	CG1	VAL B	56	44.131		-2.541	1.00	102.53
60	3484	CG2	VAL B	56	42.749	57.246 55.704	-3.058	1.00	102.53
	3485	č	VAL B	56	41.796	55.791	-1.618	1.00	102.53
	3486	ŏ	VAL B	56		59.306	-2.748	1.00	110.45
	3487	Ň	ASN B		40.783	59.952	-2.515	1.00	110.45
	3488	CA	ASN B	57 57	42.556	59.515	-3.820	1.00	137.41
65	3489	CB		57	42.235	60.554	-4.794	1.00	137.41
00	3490	CG	ASN B	57 57	42.508	60.063	-6.216	1.00	211.36
	3491	OD1	ASN B	57	43.990	59.900	-6.493	1.00	211.36
			ASN B	57	44.776	60.825	-6.294	1.00	211.36
	3492	ND2	ASN B	57	44.379	58.721	-6.959	1.00	211.36
70	3493	C	ASN B	57	40.795	61.032	-4.667	1.00	137.41
70	3494	0	ASN B	57	39.885	60.501	-5.305	1.00	137.41
								-	

	3495	N	ALA B	58	40.608	62.038	-3.818	1.00	74.20
	3496	CA	ALA B	58	39.303	62.603	-3.561	1.00	74.20
	3497 3498	CB. C	ALA B ALA B	58	39.440	63.783	-2.609	1.00	169.14
5	3499	ŏ	ALA B	58 58	38.534 38.983	63.034 63.895	-4.817 5.570	1.00	74.20
•	3500	Ň	LYS B	59	37.366	62.433	-5.579 -5.015	1.00 1.00	74.20
	3501	CA	LYS B	59	36.507	62.766	-6.137	1.00	107.95 107.95
	3502	СВ	LYS B	59	36.037	61.485	-6.837	1.00	214.35
10	3503	CG	LYS B	59	37.184	60.618	-7.354	1.00	214.35
10	3504	CD	LYS B	59	36.703	59.292	-7.930	1.00	214.35
	3505	CE	LYS B	59	37.872	58.451	-8.432	1.00	214.35
	3506 3507	NZ C	LYS B Lys b	59 59	37.428	57.138 69.514	-8.972	1.00	214.35
	3508	ŏ	LYS B	59	35.330 34.924	63.514 63.205	-5.521 -4.397	1.00	107.95
15	3509	Ň	PHE B	60	34.798	64.502	-6.234	1.00 1.00	107.95
	3510	CA	PHE B	60	33.670	65.268	-5.716	1.00	88.51 88.51
	3511	СВ	PHE B	60	33.032	66.051	-6.845	1.00	104.07
	3512	CG	PHE 8	60	33.926	67.085	-7.419	1.00	104.07
20	3513	CD1	PHE B	60	33.803	67.477	-8.736	1.00	104.07
20	3514 3515	CD2 CE1	PHE B PHE B	60	34.893	67.682	-6.635	1.00	104.07
	3516	CE2	PHE B	60 60	34.629 35.725	68.451 68.654	·9.266	1.00	104.07
	3517	CZ	PHE B	60	35.592	69.038	-7.155 -8.473	1.00	104.07
	3518	č	PHE B	60	32.616	64.397	-5.032	1.00 1.00	104.07 88.51
25	3519	0	PHE B	60	31.988	64.816	-4.060	1.00	88.51
	3520	N	GLU B	61	32.438	63.177	-5.536	1.00	122.82
	3521	CA	GLU B	61	31.453	62.251	-4.988	1.00	122.82
	3522	CB	GLU B	61	31.362	60.981	-5. 83 8	1.00	242.03
30	3523 3524	CD	GLU B	61	30.921	61.202	-7.268	1.00	242.03
50	3525	OE1	GLU B GLU B	61 61	31.866 33.080	62.107	-8.030	1.00	242.03
	3526	OE2	GLU B	61	31.395	61.812 63.111	-8.056 -8.604	1.00	242.03
	3527	c c	GLU B	61	31.772	61.856	-3.563	1.00 1.00	242.03 122.82
	3528	Ō	GLU B	61	30.884	61.426	-2.829	1.00	122.82
35	3529	N	ASP B	62	33.038	61.982	-3.173	1.00	75.67
	3530	CA	ASP B	62	33.435	61.622	-1.821	1.00	75.67
	3531	CB	ASP B	62	34.954	61.524	-1.708	1.00	186.17
	3532 3533	CG OD1	ASP B ASP B	62	35.544	60.572	-2.723	1.00	186.17
40	3534	OD2	ASP B	62 62	34.918 36.638	59.528 60.860	-2.996 -3.242	1.00	186.17
	3535	C	ASP B	62	32.889	62.643	-3.242 -0.834	1.00 1.00	186.17 75.67
	3536	Ö	ASP B	62	32.765	62.359	0.354	1.00	75.67 75.67
	3537	N	SER B	63	32.553	63.832	-1.330	1.00	56.90
4 =	3538	CA	SER B	63	31.993	64.872	-0.471	1.00	56.90
45	3539	CB	SER B	63	31.659	66.117	-1.286	1.00	0.16
	3540 3541	og	SER B	63	32.823	66.739	-1.783	1.00	80.16
	3542	C	SER B SER B	63 63	30.710 29.919	64.291	0.102	1.00	56.90
	3543	Ň	GLY B	64	30.482	63.744 64.385	-0.643 1.407	1.00	56.90
50	3544	ĈA	GLY B	64	29.254	63.819	1.941	1.00 1.00	91.31 91.31
	3545	C	GLY B	64	29.177	63.712	3.447	1.00	91.31
	3546	0	GLY B	64	30.012	64.259	4.164	1.00	91.31
	3547	N.	GLU B	65	28.154	63.014	3.922	1.00	66.19
55	3548	CA	GLU B	65	27.919	62.813	5.351	1.00	66.19
JJ	3549 3550	CB	GLU B	65 65	26.443	63.045	5.642	1.00	102.59
	3550 3551	CG CD	GLU B GLU B	65 65	25.981	62.639	7.018	1.00	122.59
	3552	OE1	GLU B	65	24.468 23.856	62.585 61.738	7.107 6.417	1.00	122.59
	3553	OE2	GLU B	65	23.890	63.390	6.417 7.863	1.00 1.00	122.59 122.59
60	3554	C	GLU B	65	28.311	61.374	5.711	1.00	66.19
	3555	0	GLU B	65	27.826	60.434	5.088	1.00	66.19
	3556	N	TYR B	66	29.183	61.182	6.697	1.00	58.72
	3557	CA	TYR B	66	29.603	59.833	7.060	1.00	58.72
65	3558 3559	CB CC	TYR B	66 66	31.093	59.680	6.855	1.00	55.88
J	3560	CG CD1	TYR B TYR B	66 66	31.576	59.790	5.452	1.00	55.88
	3561	CE1	TYR B	66 66	31.703 32.243	61.020	4.825	1.00	55.88
	3562	CD2	TYR B	66	31.986	61.109 58.657	3.548 4.772	1.00	55.88 55.88
	3563	CE2	TYR B	66	32.521	58.726	3.505	1.00 1.00	55.88 55.88
70	3564	CZ	TYR B	66	32.655	59.947	2.896	1.00	55.88
							-		30.00

	3565	ОН	TYR B	66	33.230	59.979	1.643	1.00	55.88
	3566	C	TYR B	66	29.320	59.544	8.522	1.00	58.72
	3567	0	TYR B	66	29.111	60.482	9.311	1.00	58.72
5	3568	N	LYS B	67	29.347	58.257	8.884	1.00	128.26
3	3569 3570	CA CB	LYS B	67	29.129	57.823	10.269	1.00	128.26
	3570 3571	CG	LYS B	67 67	27.689	58.067	10.679	1.00	129.32
	3572	CD	LYS B	67	26.702 25.301	57.535 57.905	9.689	1.00	129,32
	3573	CE	LYS B	67	24.314	57.545	10.098 9.007	1.00 1.00	129.32
10	3574	NZ	LYS B	67	22.936	57.963	9.372	1.00	129.32 129.32
	3575	C	LYS B	67	29.460	56.351	10.466	1.00	128.26
	3576	0	LYS B	67	29.434	55.570	9.516	1.00	128.26
	3577	N	CYS B	68	29.793	55.971	11.696	1.00	93.88
15	3578 3579	CA C	CYS B	68	30.107	54.581	11.964	1.00	93.88
13	3580	ŏ	CYS B	68 68	29.262 28.693	54.113	13.122	1.00	93.88
	3581	СВ	CYS B	68	31.609	54.923 54.381	13.850 12.247	1.00 1.00	93.88
	3582	SG	CYS B	68	32.359	55.270	13.646	1.00	200.62 200.62
••	3583	N	GLN B	69	29.148	52.797	13.255	1.00	198.52
20	3584	CA	GLN B	69	28.375	52.172	14.318	1.00	198.52
	3585	CB	GLN B	69	26.897	52.107	13.926	1.00	207.53
	3586 3587	CG CD	GLN B	69	26.082	51.114	14.734	1.00	207.53
	3588	OE1	GLN B	69 69	24.654 24.419	50.983	14.233	1.00	207.53
25	3589	NE2	GLN B	66 09	23.692	50.759 51.117	13.044 15.143	1.00	207.53
	3590	C	GLN B	69	28.921	50.768	14.527	1.00 1.00	207.53 198.52
	3591	0	GLN B	69	29.474	50.173	13.600	1.00	198.52
	3592	Ŋ	HIS B	70	28.772	50.240	15.739	1.00	126.14
30	3593	CA	HIS B	70	29.266	48.903	16.020	1.00	126.14
30	3594 3595	CB	HIS B	70	30.134	48.915	17.265	1.00	193.31
	3596	CG CD2	HIS B	70 70	31.435	49.650	17.083	1.00	193.31
	3597	ND1	HIS B	70 70	31.809 32.502	50.892 49.089	17.450 16.411	1.00 1.00	193.31
	3598	CE1	HIS B	70	33.480	49.982	16.371	1.00	193.31 193.31
35	3599	NE2	HIS B	70	33.095	51.074	16.992	1.00	193.31
	3600	Ç	HIS B	70	28.144	47.890	16.193	1.00	126.14
	3601	0	HIS B	70	26.974	48.180	15.915	1.00	126.14
	3602 3603	N CA	GLN B	71	28.511	46.697	16.639	1.00	181.78
40	3604	CB	GLN B	71 71	27.558 28.277	45.621	16.836	1.00	181.78
. •	3605	ČĞ	GLN B	71	27.687	44.424 43.082	17.456 17.057	1.00 1.00	249.38
	3606	CD	GLN B	71	27.525	42.946	15.553	1.00	249.38 249.38
	3607	OE1	GLN B	71	28.501	42.814	14.816	1.00	249.38
45	3608	NE2	GLN B	71	26.283	42.994	15.091	1.00	249.38
43	3609 3610	C	GLN B	71	26.374	46.062	17.711	1.00	181.78
	3611	0 N	GLN B	71 72	25.214	45.948 46.588	17.300	1.00	181.78
	3612	ĞA	GLN B	72 72	26.666 25.627	46.582 47.029	18.902 19.838	1.00	249.48
	3613	CB	GLN B	72	25.631	46.132	21.084	1.00 1.00	249.48 225.39
50	3614	CG	GLN B	72	24.511	46.421	22.083	1.00	225.39
	3615	CD	GLN B	72	24.526	45.478	23.273	1.00	225.39
	3616	OE1	GLN B	72	24.436	44.260	23.115	1.00	225.39
	3617 3618	NE2	GLN B	72	24.641	46.038	24.471	1.00	225.39
55	3619	C O	GLN B	72 72	25.812	48.487	20.262	1.00	249.48
-	3620	Ň	VAL B	72 73	25.935 25.821	48.787 49.395	21.455 19.288	1.00	249.48
	3621	CA	VAL B	73	26.005	50.817	19.583	1.00 1.00	181.22 181.22
	3622	CB	VAL B	73	27.465	51.205	19.481	1.00	249.28
60	3623	CG1	VAL B	73	27.738	52.552	20.109	1.00	249.28
60	3624	CG2	VAL B	73	28.193	50.235	20.151	1.00	249.28
	3625 3626	C O	VAL B	73	25.240	51.690	18.626	1.00	181.22
	3627	Ň	VAL B ASN B	73 74	25.071	51.348 53.836	17.462	1.00	181.22
_	3628	CA ·	ASN B	74 74	24.776 24.042	52.826 53.744	19.122 18.278	1.00	246.14
65	3629	СВ	ASN B	74	23.201	54.681	19.141	1.00 1.00	246.14 197.13
	3630	CG	ASN B	74	22.296	53.925	20.082	1.00	197.13
	3631	OD1	ASN B	74	21.682	52.931	19.688	1.00	197.13
	3632 3633	ND2	ASN B	74	22.202	54.394	21.324	1.00	197.13
70	3634	C O	ASN B ASN B	74 74	25.027	54.526 65.081	17.418	1.00	246.14
		•	7011 0	/ ** .	26.004	55.081	17.922	1.00	246.14

	3635	N	GLU B	75 .	24.761	54.542	16.114	1.00	146.48
	3636	CA	GLU B	75	25.597	55.232	15.135	1.00	
	3637	CB	GLU B	75	24.848	55.331			146.48
	3638	CG	GLU B				13.807	1.00	234.88
5				75	23.346	55.500	13. 96 6	1.00	234.88
,	3639	CD	GLU B	75	22.604	55.365	12.648	1.00	234.88
	3640	OE1	GLU B	75	22.784	54.328	11.970	1.00	234.88
	3641	OE2	GLU B	75	21.840	56.291	12.295	1.00	
	3642	С	GLU B	75	26.075	56.613	15.579		234.88
	3643	ŏ	GLU B	75	25.344			1.00	146.48
10	3644	Ň				57.361	16.239	1.00	146.48
10			SER B	76	27.311	56.939	15.201	1.00	102.01
	3645	CA	SER B	76	27.958	58. 20 0	15.564	1.00	102.01
	3646	CB	SER B	76	29.420	58.153	15.147	1.00	220.64
	3647	OG	SER B	76	29.501	58.098	13.732	1.00	
	3648	С	SER B	76	27.336	59.426	14.930		220.64
15	3649	ō	SER B	76				1.00	102.01
	3650	Ň			26.652	59.332	13.921	1.00	102.01
			GLU B	77	27.604	60.583	15.522	1.00	133.62
	3651	CA	GLU B	77	27.102	61.838	14.988	1.00	133.62
	3652	CB	GLU B	77	27.429	62.993	15.941	1.00	240.61
	3653	CG	GLU B	77	26.732	62.894	17.288	1.00	240.61
20	3654	CD	GLU B	77	25.218	62.995	17.179	1.00	
	3655	OE1	GLU B	77	24.686				240.61
	3656	OE2	GLU B			62.847	16.060	1.00	240.61
				<u>77</u>	24.558	63.213	18.217	1.00	240.61
	3657	Ç	GLU B	7 7	27.798	62.057	13.651	1.00	133.62
~ ~	3658	0	GLU B	77	29.023	62.177	13.597	1.00	133.62
25	3659	· N	PRO B	78	27.030	62.096	12.549	1.00	89.52
	3660	CD	PRO B	78	25.577	61.836	12.507		
	3661	CA	PRO B	78	27.543			1.00	87.18
	3662	CB				62.294	11.196	1.00	89.52
			PRO B	78	26.295	62.633	10.408	1.00	87.18
20	3663	CG	PRO B	78	25.313	61.698	11.009	1.00	87.18
30	3664	С	PRO B	78	28.586	63.370	11.098	1.00	89.52
	3665	0	PRO B	78	28.644	64.258	11.943	1.00	89.52
	3666	N	VAL B	79	29.430	63.270	10.082	1.00	
	3667	CA	VAL B	79	30.475	64.256			99.13
	3668	CB					9.872	1.00	99.13
35				79	31.833	63.720	10.291	1.00	115.84
23	3669	CG1	VAL B	79	32.929	64.618	9.749	1.00	115.84
	3670	CG2	VAL B	79	31.908	63.671	11.798	1.00	115.84
	3671	С	VAL B	79	30.512	64.571	8.401	1.00	99.13
	3672	0	VAL B	79	30.573	63.654	7.592	1.00	99.13
	3673	N	TYR B	80	30.480	65.853	8.044	1.00	
40	3674	CA	TYR B	80					70.58
	3675				30.490	66.213	6.637	1.00	70.58
		CB	TYR B	80	29.622	67.426	6.352	1.00	173.93
	3676	CG	TYR B	80	29.319	67.524	4.884	1.00	173.93
	3677	CD1	TYR B	80	28.546	66.550	4.261	1.00	173.93
	3678	CE1	TYR B	80	28.266	66.604	2.913	1.00	173.93
45	3679	CD2	TYR B	80	29.824	68.559	4.106	1.00	
	3680	CE2	TYR B	80	29.561	68.613			173.93
	3681	CZ	TYR B				2.729	1.00	173.93
				80	28.769	67.630	2.148	1.00	173.93
	3682	ОН	TYR B	80	28.432	67.702	0.811	1.00	173.93
5 0	3683	С	TYR B	<u>:</u> 0	31.858	66.511	6.103	1.00	70.58
50	3684	0	TYR B	80	32.657	67.183	6.739	1.00	70.58
	3685	N	LEU B	81	32.109	66.033	4.902	1.00	86.81
	3686	CA	LEU B	81	33.375	66.256			
	3687	CB	LEU B				4.254	1.00	86.81
				81	34.030	64.899	3.970	1.00	52.23
55	3688	CG	LEU B	81	35.301	65.038	3.148	1.00	52.23
55	3689	CD1	LEU B	81	36.303	65.810	3.970	1.00	52.23
	3690	CD2	LEU B	81	35.843	63.724	2.783	1.00	52.23
	3691	С	LEU B	81	33.090	66.999	2.944	1.00	
	3692	Ö	LEU B	81	32.240				86.81
	3693	Ň	GLU B			66.576	2.171	1.00	86.81
60				82	33.777	68.104	2.682	1.00	81.52
UU	3694	CA	GLU B	82	33.537	68.808	1.430	1.00	81.52
	3695	CB	GLU B	82	33.000	70.212	1.700	1.00	166.15
	3696	CG	GLU B	82	32.168	70.757	0.552	1.00	166.15
	3697	CD	GLU B	82	31.619	72.139	0.827		
	3698	ÖE1	GLU B					1.00	166.15
65				82	31.239	72.409	1.988	1.00	166.15
JJ	3699	OE2	GLU B	82	31.557	72.953	-0.118	1.00	166.15
	3700	Ç	GLU B	82	34.800	68.898	0.584	1.00	81.52
	3701	0	GLU B	82	35.856	69.283	1.072	1.00	81.52
	3702	N	VAL B	83	34.691	68.555	-0.692	1.00	81.14
	3703	CA	VAL B	83	35.842	68.595			
70	3704	CB	VAL B				-1.584	1.00	81.14
	0,07	J D	AWF D	83	35.910	67.346	-2.417	1.00	54.13

	3705	CG1	VAL B	83-	37.014	67.472	-3.433	1.00	E4 40
	3706	CG2	VAL B	83	36.159	66.136	-1.512	1.00	54.13 54.13
	3707	С	VAL B	83	35.848	69.781	-2.535	1.00	81.14
_	3708	Ο.	VAL B	83	34.831	70.075	-3.168	1.00	81.14
5	3709	N	PHE B	84	37.000	70.441	-2.667	1.00	61.79
	3710	CA	PHE B	84	37 084	71.612	-3.530	1.00	61.79
	3711	CB	PHE B	84	37.407	72.864	-2.729	1.00	77.82
	3712	CG	PHE B	84	36.432	73.162	-1.660	1.00	77.82
10	3713	CD1	PHE B	84	36.408	72.410	-0.500	1.00	77.82
10	3714	CD2	PHE B	84	35.555	74.223	-1.790	1.00	77.82
	3715	CE1	PHE B	84	35.513	72.699	0.522	1.00	77.82
	3716	CE2	PHE B	84	34.650	74.529	-0.779	1.00	77.82
	3717	CZ	PHE B	84	34.634	73.766	0.384	1.00	77.82
15	3718	C	PHE B	84	38.081	71.568	-4.654	1.00	61.79
13	3719	0	PHE B	84	38.978	70.728	-4.701	1.00	61.79
	3720 3721	N CA	SER B	8 5	37.893	72.538	-5.543	1.00	129.28
	3722	CB	SER B	8 5	38.736	72.777	-6.696	1.00	129.28
	3723	OG	SER B SER B	85 85	38.066	72.284	-7.980	1.00	132.41
20	3724	C	SER B	85 85	38.879	72.526	-9.116	1.00	132.41
20	3725	ŏ	SER B	85	38.840	74.296	-6.713	1.00	129.28
	3726	Ň	ASP B	86	37.845 40.026	74.988	-6.967	1.00	129.28
	3727	CA	ASP B	86	40.026	74.811	-6.395	1.00	77.53
	3728	CB	ASP B	86	39.348	76.257 76.933	-6.385	1.00	77.53
25	3729	CG	ASP B	86	38.874	78.300	-5.354 5.900	1.00	206.86
	3730	OD1	ASP B	86	39.733	79.139	-5.809 -6.163	1.00	206.86
	3731	OD2	ASP B	86	37.644	78.535	-5.812	1.00	206.86
	3732	C	ASP B	86	41.719	76.537	-6.065	1.00 1.00	206.86
	3733	ō	ASP B	86	42.423	75.643	-5.601	1.00	77.53
30	3734	N	TRP B	87	42.186	77.759	-6.313	1.00	77.53
	3735	CA	TRP B	87	43.589	78.072	-6.048	1.00	63.09 63.09
	3736	CB	TRP B	87	43.934	79.488	6.505	1.00	213.86
	3737	CG	TRP B	87	44.332	79.502	-7.919	1.00	213.86
~~	3738	CD2	TRP B	87	43.467	79.711	-9.031	1.00	213.86
35	3739	CE2	TRP B	87	44.225	79.492	-10.196	1.00	213.86
	3740	CE3	TRP B	87	42.115	80.053	-9.157	1.00	213.86
	3741	CD1	TRP B	87	45.561	79.186	-8.435	1.00	213.86
	3742	NE1	TRP B	87	45.500	79.175	-9.807	1.00	213.86
40	3743	CZ2	TRP B	87	43.674	79.604	-11.468	1.00	213.86
40	3744	CZ3	TRP B	87	41.570	80.162	-10.423	1.00	213.86
	3745	CH2	TRP B	87	42.347	79.943	-11.559	1.00	213.86
	3746	C	TRP B	87	43.913	77.935	-4.589	1.00	63.09
	3747 3 748	0	TRP B	87	44.856	77.221	-4.208	1.00	63.09
45	3748 3749	N CA	LEU B	88	43.110	78.622	-3.783	1.00	95.94
73	3750	CB	LEU B LEU B	88	43.280	78.617	-2.349	1.00	95.94
	3751	ÇG	LEU B	88	43.600	80.021	-1.861	1.00	93.07
	3752	CD1	LEU B	88 88	44.931 45.167	80.558	-2.325	1.00	93.07
	3753	CD2	LEU B	88	46.019	81.882	-1.668	1.00	93.07
50	3754	Č	LEU B	88	42.050	79.559 78.126	-1.955 -1.621	1.00	93.07
	3755	ŏ	LEU B	88	40.927	78.425	-2.004	1.00	95.94
	3756	Ň	LEU B	89	42.276	77.380	-0.550	1.00 1.00	95.94
	3757	CA	LEU B	89	41.191	76.863	0.265	1.00	57.56
	3758	CB	LEU B	89	41.063	75.370	0.059	1.00	57.56 98.29
55	3759	CG	LEU B	89	39.972	74.802	0.940	1.00	98.29
	3760	CD1	LEU B	89	38.700	75.640	0.767	1.00	98.29
	3761	CD2	LEU B	89	39.741	73.357	0.564	1.00	98.29
	3762	С	LEU B	89	41.488	77.138	1.724	1.00	57.56
<i>c</i> 0	3763	0	LEU B	89	42.566	76.832	2.192	1.00	57.56
60	3764	N	LEU B	90	40.553	77.737	2.444	1.00	82.03
	3765	CA	LEV B	90	40.787	78.008	3.857	1.00	82.03
	3766	CB	LEU B	90	40.005	79.244	4.303	1.00	51.54
	3767	CG	LEV B	90	40.073	79.537	5.807	1.00	51.54
65	3768	CD1	LEU B	90	41.486	79.805	6.154	1.00	51.54
UJ	3769	CD2	LEU B	90	39.203	80.720	6.203	1.00	51.54
	3770	C	LEU B	90	40.347	76.808	4.674	1.00	82.03
	3771	0	LEU B	90	39.173	76.431	4.667	1.00	82.03
	3772 3773	N CA	GLN B	91	41.274	76.199	5.391	1.00	55.00
70	3773 3774	CA CB	GLN B	91	40.904	75.024	6.182	1.00	55.00
	3//4	OB	GLN B	91	41.909	73.900	5.955	1.00	79.62

	3775	CG	GLN B	91-	42.017	73.500	4.501	1.00	79.62
	3776	CD	GLN B	91	42.871	72.287	4.316	1.00	79.62
	3777	OE1	GLN B	91	44.072	72.334	4.524	1.00	79.62
_	3778	NE2	GLN B	91	42.253	71.180	3.942	1.00	79.62
5	3779	C	GLN B	91	40.793	75.316	7.670	1.00	55.00
	3780	0	GLN B	91	41.552	76.118	8.212	1.00	55.00
	3781	N	ALA B	92	39.846	74.680	8.344	1.00	72.63
	3782	CA	ALA B	92	39.692	74.939	9.760	1.00	72.63
10	3783	CB	ALA B	92	38.406	75.678	10.004	1.00	131.49
10	3784	C	ALA B	92	39.691	73.632	10.519	1.00	72.63
	3785	0	ALA B	92	39.122	72.634	10.050	1.00	72.63
	3786	N	SER B	93	40.338	73.624	11.685	1.00	73.84
	3787	CA CB	SER B	93	40.381	72,421	12.512	1.00	73.84
15	3788	OG	SER B	93	41.018	72.709	13.873	1.00	152.84
15	3789 3790	C	SER B SER B	93	40.445	73.845	14.491	1.00	152.84
	3790	ŏ	SER B	93 93	38.934	72.013	12.691	1.00	73.84
	3792	N	ALA B	93 94	38.515 38.167	70.973	12.179	1.00	73.84
	3793	CA	ALA B	94 94	36.743	72.859	13.378	1.00	105.05
20	3794	CB	ALA B	94	36.517	72.624 72.246	13.619	1.00	105.05
20	3795	Č	ALA B	94	35.978	73.898	15.061 13.280	1.00 1.00	185.57
	3796	ŏ	ALA B	94	36.478	74.988	13.524	1.00	105.05
	3797	Ň	GLU B	95	34.776	73.763	12.724	1.00	105.05
	3798	CA	GLU B	95	34.005	74.936	12.340	1.00	101.72
25	3799	CB	GLU B	95	33.081	74.601	11.175	1,00	101.72 160.65
	3800	CG	GLU B	95	33.822	74.120	9.941	1.00	160.65
	3801	CD	GLU B	95	32.955	74.120	8.692	1.00	160.65
	3802	OE1	GLU B	95	33.455	73.705	7.625	1.00	160.65
	3803	OE2	GLU B	95	31.779	74.538	8.771	1.00	160.65
30	3804	C	GLU B	95	33.205	75.550	13.473	1.00	101.72
	3805	0	GLU B	95	32.732	76.677	13.354	1.00	101.72
	3806	N	VAL B	96	33.050	74.807	14.565	1.00	87.11
	3807	CA	VAL B	96	32.322	75.296	15.730	1.00	87.11
	3808	CB	VAL B	96	30.947	74.746	15.781	1.00	166.75
35	3809	CG1	VAL B	96	30.147	75. 5 95	16.714	1.00	166.75
	3810	CG2	VAL B	96	30.349	74.728	14.367	1.00	168.75
	3811	C	VAL B	96	33.096	74.866	16.955	1.00	87.11
	3812	0	VAL B	96	33.528	73.724	17.052	1.00	87.11
40	3813	N	VAL B	97	33.260	75.781	17.900	1.00	103.60
40	3814	CA	VAL B	97	34.080	75.505	19.067	1.00	103.60
	3815	CB	VAL B	97	35.444	76.140	18.858	1.00	67.08
	3816	CG1 CG2	VAL B	97	36.415	75.622	19.857	1.00	67.08
	3817 3818	C	VAL B VAL B	97 07	35.924	75.882	17.456	1.00	67.08
45	3819	ŏ	VAL B	97	33.591	76.003	20.417	1.00	103.60
13	3820	N	MET B	97 98	33.142 33.730	77.136 75.168	20.533	1.00	103.60
	3821	CA	MET B	98	33.341	75.100 75.542	21.441 22.798	1.00 1.00	173.13
	3822	CB	MET B	98	33.361	74.306	23.696	1.00	173.13
	3823	CG	MET B	98	32.369	73.237	23.290	1.00	240.86 240.86
50	3824	SD	MET B	98	30.722	73.639	23.866	1.00	240.86
	3825	CE	MET B	98	30.921	73.267	25.612	1.00	240.86
	3826	C	MET B	98	34.341	76.573	23.323	1.00	173.13
	3827	0	MET B	98	35.547	76.380	23.185	1.00	173.13
	3828	N	GLU B	99	33.849	77.658	23.918	1.00	116.59
55	3829	CA	GLU B	99	34.731	78.695	24.451	1.00	116.59
	3830	CB	GLU B	99	33.954	79.631	25.376	1.00	249.41
	3831	CG	GLU B	99	34.610	80.985	25.567	1.00	249.41
	383 2	CD	GLU B	99	34.016	81.763	26.727	1.00	249.41
60	3833	OE1	GLU B	99	32.782	81.690	26.920	1.00	249.41
60	3834	OE2	GLU B	99	34.781	82.455	27.435	1.00	249.41
	3835	Č	GLU B	99	35. 85 3	78.023	25.247	1.00	116.59
	3836	0	GLU B	99	35.582	77.203	26.127	1.00	116.59
	3837	N	GLY B	100	37.106	78.351	24.935	1.00	84.75
65	3838	CA	GLY B	100	38.221	77.751	25.651	1.00	84.75
O)	3839	C	GLY B	100	39.031	76.722	24.883	1.00	84.75
	3840	O .	GLY B	100	40.171	76.451	25.243	1.00	84.75
	3841 3842	N CA	GLN B	101	38.464	76.151	23.824	1.00	108.09
	3842 3843	CB	GLN B GLN B	101	39.167	75.134 74.221	23.033	1.00	108.09
70	3844	CG	GLN B	101 101	38.151	74.231 72.307	22.324	1.00	249.17
, ,	30-7	~~	GL1 D	101	37.313	73.397	23.267	1.00	249.17

	3845 3846 3847 3848 5 3849 3850 3851	OE NE	E1 GLN E2 GLN GLN GLN PRO	1 B 1 B 1 B 1 B	101 34 101 40 101 40 101 40	8.163 72.6 9.643 73.2 9.370 71.3 0.159 75.6 0.186 76.8 0.996 74.8	192 25 195 24 187 22 180 21	5.255 1. 4.094 1. 2.000 1. 1.723 1.	00 108.09
	3852 3853 3854 3855 3856	CA CB CG C	PRO PRO PRO PRO	8 8 8	102 41 102 43 102 42	.175 73.37 .948 75.30 .006 74.21 .177 72.97	71 21 01 20 12 20 19 20	.422 1.0 .665 1.0 .429 1.0 .431 1.0 .592 1.0	00 84.30 00 171.21 00 84.30 00 171.21
	3857 3858 3859 3860	O N CA CB CG	LEU	B B B	102 40. 103 41. 103 41. 103 40.	260 74.79 828 76.35 299 76.58 437 77.83	6 19. 9 18. 1 18. 8 16.	051 1.0 745 1.0 228 1.0 900 1.0	0 84.30 0 84.30 0 75.78
2	3861 3862 3863 20 3864 3865	CD1 CD2 C O N	LEU LEU (LEU (B 1	103 39.1 103 38.9 103 39.1 103 42.4 103 43.2	942 76.897 117 79.391 111 76.793	3 15.5 7 15.1 15.4 15.8	515 1.00 142 1.00 183 1.00 192 1.00	79.40 79.40 79.40
2	3866 3867 3868 3869 3870	CA CB CG CD1 CD2	PHE E PHE E PHE B PHE B	3 1 3 1	04 42.4 04 43.5 04 44.4 04 45.0 04 44.3	70 75.993 24 76.182 41 74.953 88 74.577	14.8	28 1.00 38 1.00 52 1.00	75.78 73.92 73.92 179.34
3	3871 3872 3873	CE1 CE2 CZ C	PHE B PHE B PHE B PHE B	10	04 46.42 04 44.96 04 47.02 04 46.29	74.880 73.550 8 74.527 73.857	16.03 15.29 17.24 16.51 17.48	35 1.00 9 1.00 8 1.00 2 1.00	179.34 179.34 179.34 179.34 179.34
35	3876 3877 3878	O N CA CB CG	PHE B LEU B LEU B LEU B	10 10 10 10 10	42.12 5 43.38 5 42.98 5 42.50	1 75.717 7 77.581 5 77.920 3 79.354	12.44 11.94 11.830 10.468 10.385	8 1.00 7 1.00 8 1.00 1.00	179.34 73.92 73.92 49.92 49.92
40	3881 3882 3883 3884	CD1 CD2 C O N	LEU B LEU B LEU B LEU B ARG B	105 105 105 105	40.828 40.368 44.224 45.327	81.064 78.612 77.773	11.381 11.137 11.223 9.580 9.991	1.00 1.00 1.00	78.62 78.62 78.62 78.62 49.92
45	3885 3886 3887 3888 3889	CA CB CG CD NE	ARG B ARG B ARG B ARG B ARG B	106 106 106 106	45.195 45.537	77.317 77.131 75.649 75.284 73.775	8.355 7.494 7.475 6.526	1.00 1.00 1.00 1.00 1.00	49.92 79.70 79.70 126.47 126.47
50	3890 3891 3892 3893 3894	CZ NH1 NH2 C	ARG B ARG B ARG B ARG B	106 106 106 106 106	47.760 47.802 46.869 48.768 44.900	73.414 72.255 71.343 72.018	6.383 5.412 4.773 5.006 3.891	1.00 1.00 1.00 1.00 1.00	126.47 126.47 126.47 126.47
55	3895 3896 3897 3898 3899	O N CA C	ARG B CYS B CYS B CYS B CYS B	106 107 107 107 107	43.899 45.730 45.507 46.217	77.615 77.192 78.518 78.971 77.938	6.083 5.483 5.553 4.177 3.331	1.00 1.00 1.00 1.00	126.47 79.70 79.70 64.58 64.58
60	3900 3901 3902 3903 3904	CB SG N CA CB	CYS B CYS B HIS B HIS B	107 107 108 108 108	47.442 46.087 45.402 45.435 45.970	77.869 80.353 81.142 77.124 76.037	3.318 3.919 2.422 2.639 1.845	1.00 1.00 1.00 1.00 1.00	64.58 64.58 107.35 107.35 77.57
65	3905 3906 3907 3908	OG CD2 ND1 CE1 NE2	HIS B HIS B HIS B HIS B	108 108 108 108	45.151 45.702 45.138 46.977 47.170	74.790 73.548 72.631 73.098 71.951	2.131 1.513 0.691 1.776	1.00 1.00 1.00 1.00 1.00	77.57 100.22 100.22 100.22 100.22
	3909 3910 3911 3912 3913	C O N CA C	HIS B HIS B GLY B GLY B	108 108 108 109 109	46.070 46.002 44.981 47.180 47.338	71.645 76.296 76.659 76.079	1.149 0.483 0.352 -0.262 -0.231	1.00 1.00 1.00 1.00 1.00	100.22 100.22 77.57 77.57
70	3914	ŏ	GLY B	109 109	47.018 47.115	76.303 75.057. 73.962	-1.652 -2.430 -1.886	1.00 1.00 1.00	82.92 82.92 82.92 82.92

	3915 3916	N CA	TRP B	110	46.628	75.221	-3.692	1.00	89.13
	3917	CB	TRP B	110	46.294	74.086	-4.536	1.00	89.13
	3918	CG	TRP B	110 110	45.749 45.538	74.564 73.457	-5.874	1.00	136.31
5	3919	· CD2	TRP B	110	44.323	73.457 72.730	-6.838 -7.054	1.00	136.31
•	3920	CE2	TRP B	110	44.590	71.748	-8.028	1.00 1.00	136.31
	3921	CE3	TRP B	110	43.025	72.815	-6.517	1.00	136.31 136.31
	3922	CD1	TRP B	110	46.464	72.907	·7.659	1.00	136.31
	3923	NE1	TRP B	110	45.908	71.879	-8.380	1.00	136.31
10	3924	CZ2	TRP B	110	43.615	70.853	-8.484	1.00	136.31
	3925	CZ3	TRP B	110	42.052	71.923	-6.969	1.00	136.31
	3926 3927	CH2	TRP B	110	42.356	70.954	-7.943	1.00	136.31
	3928	C O	TRP B	110 110	47.525 48.662	73.218 73.698	-4.759 4.730	1.00	89.13
15	3929	Ň	ARG B	111	47.294	71.927	-4.730 -4.960	1.00 1.00	89.13
	3930	CA	ARG B	111	48.376	70.980	-5.192	1.00	107.42 107.42
	3931	CB	ARG B	111	48.900	71.128	-6.598	1.00	249.40
	3932	CG	ARG B	111	48.148	70.283	-7.546	1.00	249.40
20	3933	CD	ARG B	111	48.856	70.281	-8.825	1.00	249.40
20	3934 3935	NE CZ	ARG B	111	48.857	68.940	-9.379	1.00	249.40
	3936	CZ NH1	ARG B	111 111	49.507 50.222	67.898	-8.8 62	1.00	249.40
	6 937	NH2	ARG B	111	49.435	68.039 66.714	-7.753 -9.465	1.00 1.00	249.40
•	3938	C	ARG B	111	49.528	71.110	-4.2 3 7	1.00	249.40 107.42
25	3939	Ó	ARG B	111	50.645	70.724	-4.550	1.00	107.42
	3940	N	ASN B	112	49.249	71.676	-3.075	1.00	103.89
	3941	CA	ASN B	112	50.250	71.869	-2.050	1.00	103.89
	3942	CB	ASN B	112	50.805	70.525	-1.599	1.00	101.72
30	3943 3944	CG OD1	ASN B	112	51.387	70.592	-0.214	1.00	101.72
50	3945	ND2	ASN B	112 112	51.759 51.479	71.673 69.442	0.261	1.00	101.72
	3946	C	ASN B	112	51.405	72.778	0.449 -2.470	1.00 1.00	101.72 103.89
	3947	ō	ASN B	112	52.504	72.698	-1.905	1.00	103.89
2-	3948	N	TRP B	113	51.177	73.636	-3.460	1.00	84.24
35	3949	CA	TRP B	113	52. 23 2	74.553	-3.854	1.00	84.24
	3950	CB	TRP B	113	51.806	75.411	-5.031	1.00	165.30
	3951 3952	CG CD2	TRP B	113	51.859	74.694	-6.297	1.00	165.30
	3953	CE2	TRP B	113 113	50.952 51.420	74.827 73.995	-7.383 -8.423	1.00	165.30
40	3954	CE3	TRP B	113	49.785	75.580	-7.589	1.00 1.00	165.30 165.30
	3955	CD1	TRP B	113	52.816	73.805	-6.695	1.00	165.30
	3956	NE1	TRP B	113	52.561	73.380	-7.973	1.00	165.30
	3957	CZ2	TRP B	113	50.763	73.890	-9.652	1.00	165.30
45	3958 3959	CZ3	TRP 8	113	49.128	75.478	-8.808	1.00	165.30
73	3960	CH2	TRP B	113 113	49.619 52.597	74.834 75.473	-9.826	1.00	165.30
	3961	ŏ	TRP B	113	52.387 52.201	75.473 75.258	-2.697 -1.543	1.00 1.00	84.24
	3962	Ň	ASP B	114	53.370	76.501	-3.013	1.00	84.24 127.07
	3963	CA	ASP B	114	53.773	77.459	-2.006	1.00	127.07
50	3964	CB	ASP B	114	55.289	77.629	-2.007	1.00	190.00
	3965	CG	ASP B	114	55.992	76.535	-1.236	1.00	190.00
	3966	OD1	ASP B	114	55.702	76.387	-0.030	1.00	190.00
	3967 3968	OD2 C	ASP B	114 114	56.831 53.098	75.825 79.704	-1.829	1.00	190.00
55	3969	ŏ	ASP B	114	52.985	78.794 79.253	-2.255 -3.402	1.00	127.07
	3970	Ň	VAL B	115	52.641	79.406	-1.165	1.00 1.00	127.07 97.38
	3971	CA	VAL B	115	51.969	80.696	-1.229	1.00	97.38
	3972	CB	VAL B	115	50.571	80.635	-0.623	1.00	112.10
60	3973	CG1	VAL B	115	49.833	81.905	-0.946	1.00	112.10
oo	3974 3075	CG2	VAL B	115	49.830	79.436	-1.155	1.00	112.10
	3975 3976	C O	VAL B	115	52.767	81.723	-0.451	1.00	97.38
	3977	N	TYR B	115 116	53.333 52.804	81.428 82.940	0.613	1.00	97.38 76.30
_	3978	CA	TYR B	116	53.547	84.019	-0.985 -0.335	1.00 1.00	76.30 76.30
65	3979	CB	TYR B	116	54.745	84.433	-0.335 -1.206	1.00	76.30 116.08
	3980	CG	TYR B	116	55.758	83.328	-1.431	1.00	116.08
	3981	CD1	TYR B	116	55.720	82.529	-2.581	1.00	116.08
	3982	CE1	TYR B	116	56.634	81.486	-2.770	1.00	116.08
70	3983 3984	CD2 . CE2	TYR B	116	56.736 57.657	83.061	-0.476	1.00	116.08
. •	J304	CEE	ITR B	116	57.657	82.024	-0.650	1.00	116.08

	3985 3986	CZ OH	TYR B TYR B	118 116	57.602 58.498	81.238 80.201	-1.798 -1.964	1.00	116.08
	3987	Č.	TYR B	116	52.654	85.227	-0.059	1.00 1.00	116.08
_	3988	ŏ.	TYR B	116	51.502	85.276	-0.514	1.00	76.30
5	3989	N	LYS B	117	53.193	86.190	0.692	1.00	76.30 87.81
	3990	CA	LYS B	117	52.463	87.411	1.036	1.00	87.81
	3991	CB	LYS B	117	52.371	88.354	-0.171	1.00	224.81
	3992	CG	LYS B	117	53.560	89.283	-0.373	1.00	224.81
10	3993 3994	CD CE	LYS B Lys b	117	53.183	90.436	-1.295	1.00	224.81
10	3995	NZ	LYS B	117 117	52.028 51.604	91.248 92.373	-0.711	1.00	224.81
	3996	· C	LYS B	117	51.059	87.049	-1.593 1.489	1.00	224.81
•	3997	Ŏ	LYS B	117	50.060	87.542	0.946	1.00 1.00	87.81
	3998	N	VAL B	118	50.983	86.194	2.498	1.00	87.81 60.09
15	3999	CA	VAL B	118	49.696	85.737	2.994	1.00	60.09
	4000	CB .	VAL B	118	49.815	84.344	3.577	1.00	85.68
	4001	CG1	VAL B	118	48.782	84.141	4.647	1.00	85.68
	4002	CG2	VAL B	118	49.604	83.325	2.485	1.00	85.68
20	4003 4004	C O	VAL B	118	49.066	86.622	4.034	1.00	60.09
20	4004	N	VAL B	118	49.752	87.066	4.963	1.00	60.09
	4006	CA	ILE B	119 119	47.753 47.003	86.837 87.686	3.901	1.00	64.26
	4007	CB	ILE B	119	46.704	89.027	4.830 4.196	1.00 1.00	64.26
	4008	CG2	ILE B	119	46.039	89.920	5.184	1.00	68.56
25	4009	CG1	ILE B	119	47.998	89.654	3.705	1.00	68.56
	4010	CD1	ILE B	119	47.766	90.828	2.843	1.00	68.56 68.56
	4011	С	ILE B	119	45.672	87.052	5.173	1.00	64.26
	4012	0	ILE B	119	44.890	86.771	4.259	1.00	64.26
30	4013	N	TYR B	120	45.402	86.803	6.458	1.00	74.17
30	4014	CA	TYR B	120	44.110	86.216	6.816	1.00	74.17
	4015 4016	CB CG	TYR B	120	44.176	85.345	8.066	1.00	67.28
	4017	CD1	TYR B TYR B	120 120	44.901	84.067	7.887	1.00	67.28
	4018	CE1	TYR B	120	46.269 46.975	84.024 82.840	8.002	1.00	67.28
35	4019	CD2	TYR B	120	44.225	82.896	7.818 7.582	1.00 1. 0 0	67.28
	4020	CE2	TYR B	120	44.909	81.695	7.390	1.00	67.28 67.28
	4021	CZ	TYR B	120	46.286	81.680	7.511	1.00	67.28
	4022	ОН	TYR B	120	46.966	80.507	7.340	1.00	67.28
40	4023	С	TYR B	120	43.185	87.348	7.125	1.00	74.17
40	4024	0	TYR B	120	43.613	88.351	7.669	1.00	74.17
	4025	N	TYR B	121	41.916	87.180	6.799	1.00	60.66
	4026 4027	CA CB	TYR B	121	40.938	88.213	7.080	1.00	60.66
	4028	CG	TYR B TYR B	121 121	40.355 41.299	88.760	5.776	1.00	108.81
45	4029	CD1	TYR B	121	42.398	89.557 88.961	4.908 4.308	1.00	108.81
	4030	CE1	TYR B	121	43.239	89.678	3.449	1.00 1.00	108.81 108.81
	4031	CD2	TYR B	121	41.058	90.900	4.640	1.00	108.81
	4032	CE2	TYR B	121	41.890	91.629	3.788	1.00	108.81
50	4033	CZ	TYR B	121	42.976	91.009	3.195	1.00	108.81
50	4034	ОН	TYR B	121	43.794	91.710	2.340	1.00	108.81
	4035	C	TYR B	121	39.781	87.692	7.936	1.00	60.66
	4036 4037	0	TYR B	121	39.301	86.560	7.736	1.00	60.66
	4038	N CA	LYS B LYS B	122	39.332	88.510	8.885	1.00	76.13
55	4039	CB	LYS B	122 122	38.1⊱⊲ 38.594	88.138	9.715	1.00	76.13
•	4040	ČĠ	LYS B	122	37.410	87.874 87.462	11.168 12.032	1.00	102.31
	4041	CD	LYS B	122	37.738	87.523	13.489	1.00 1.00	102.31 102.31
	4042	CE	LYS B	122	36.509	87.285	14.327	1.00	102.31
~	4043	NZ	LYS B	122	36.834	87.504	15.762	1.00	102.31
60	4044	С	LYS B	122	37.200	89.289	9.679	1.00	76.13
	4045	0	LYS B	122	37.507	90.390	10.145	1.00	76.13
	4046	N	ASP B	123	36.013	89.034	9.131	1.00	98.55
	4047	CA	ASP B	123	34.968	90.049	9.023	1.00	98.55
65	4048 4049	CB CG	ASP B	123	34.492	90.473	10.414	1.00	136.85
55	4050	OD1	ASP B ASP B	123 123	33.604	89.429	11.059	1.00	136.85
	4051	OD2	ASP B	123	32.692 33.810	88.925 89.122	10.363 12.256	1.00	136.85
	4052	C	ASP B	123	35.420	91.268	8.217	1.00 1.00	136.85 98.55
	4053	Ō	ASP B	123	35.168	92.418	8.597	1.00	98.55
70	4054	N	GLY B	124	36.094	90.997	7.099	1.00	109.74

	4055 4056	CA C	GLY B GLY B	124 124	36.578 37.817	92.050 92.800	6.224 6.688	1.00 1.00	109.74
	4057	ŏ	GLY B	124	38.371	93.600	5.938	1.00	109.74 109.74
_	4058	Ν.	GLU B	125	38.269	92.542	7.911	1.00	80.11
5	4059	CA	GLU B	125	39.438	93.230	8.468	1.00	80.11
	4060 4061	CB CG	GLU B GLU B	125 125	39.276	93.432	9.990	1.00	173.35
	4062	CD	GLU B	125	38.192 38.621	94.412 95.865	10.446 10.344	1.00 1.00	173.35
	4063	OE1	GLU B	125	39.591	96.256	11.030	1.00	173.35 173.35
10	4064	OE2	GLU B	125	37.982	96.615	9.577	1.00	173.35
	4065	C	GLU B	125	40.723	92.462	8.243	1.00	80.11
	4066 4067	O N	GLU B ALA B	125	40.728	91.235	8.308	1.00	80.11
	4068	CA	ALA B	126 126	41.817 43.101	93.171 92.501	7.986 7.826	1.00 1.00	116.19
15	4069	СВ	ALA B	126	44.165	93.513	7.450	1.00	116.19 157.65
	4070	С	ALA B	126	43.385	91.901	9.216	1.00	116.19
	4071	0	ALA B	126	43.051	92.516	10.227	1.00	116.19
	4072	N CA	LEU B	127	43.985	90.715	9.286	1.00	101.69
20	4073 4074	CB	LEU B LEU B	127 127	44.246 43.383	90.109 88.875	10.586	1.00	101.69
	4075	CG	LEU B	127	43.207	88.660	10.761 12.259	1.00 1.00	85.89 85.89
	4076	CD1	LEU B	127	42.594	89.929	12.853	1.00	85.89
	4077	CD2	LEU B	127	42.337	87.450	12.551	1.00	85.89
25	4078	C	LEU B	127	45.696	89.750	10.902	1.00	101.69
23	4079 4080	O N	LEU B LYS B	127 128	46.240 46.306	90.197 88.916	11.910	1.00	101.69
	4081	CA	LYS B	128	46.306 47.701	88.530	10.070 10.256	1.00 1.00	84.42
	4082	СВ	LYS B	128	47.794	87.118	10.847	1.00	84.42 200.20
20	4083	ÇG	LYS B	128	47.160	86.955	12.220	1.00	200.20
30	4084	CD	LYS B	128	47.968	87.634	13.317	1.00	200.20
	4085 4086	CE NZ	LYS B Lys b	128	47.352	87.350	14.684	1.00	200.20
	4087	C	LYS B	128 128	48.172 48.360	87.864 88.558	15.817 8.877	1.00 1.00	200.20
	4088	ŏ	LYS B	128	47.675	88.404	7.853	1.00	84.42 84.42
35	4089	N	TYR B	129	49.675	88.750	8.839	1.00	107.40
	4090	CA	TYR B	129	50.387	88.773	7.566	1.00	107.40
	4091 4092	CB CG	TYR B TYR B	129	50.519	90.208	7.067	1.00	112.63
	4093	CD1	TYR B	129 129	51.618 51.417	90.368 90.021	6.043 4.712	1.00	112.63
40	4094	CE1	TYR B	129	52.442	90.116	3.781	1.00 1.00	112.63 112.63
	4095	CD2	TYR B	129	52.879	90.814	6.422	1.00	112.63
	4096	CE2	TYR B	129	53.915	90.911	5.502	1.00	112.63
	4097 4098	CZ OH	TYR B TYR B	129	53.693	90.562	4.183	1.00	112.63
45	4099	C	TYR B	129 129	54.719 51.779	90.665 88.146	3.260 7.621	1.00	112.63
	4100	ŏ	TYR B	129	52.518	88.373	8.575	1.00 1.00	107.40 107.40
	4101	N	TRP B	130	52.138	87.376	6.587	1.00	87.42
	4102	CA	TRP B	130	53.454	86.735	6.524	1.00	87.42
50	4103	CB	TRP B	130	53.400	85.311	7.090	1.00	190.57
50	4104 4105	CG CD2	TRP B	130 130	52.744 53.401	85.171 84.954	8.423	1.00	190.57
	4106	CE2	TRP B	130	52.392	84.829	9.674 10.656	1.00 1.00	190 <i>.</i> 57 190.57
	4107	CE3	TRP B	130	54.746	84.861	10.062	1.00	190.57
E E	4108	CD1	TRP B	130	51.406	85.166	8.687	1.00	190.57
55	4109	NE1	TRP B	130	51.185	84.959	10.025	1.00	190.57
	4110 4111	CZ2 CZ3	TR⊬ B TRP B	130 130	52.686 55.041	84.607	12.010	1.00	190.57
	4112	CH2	TRP B	130	54.011	84.641 84.510	11.412 12.366	1.00 1.00	190.57 190.57
	4113	C	TRP B	130	53.968	86.652	5.085	1.00	87.42
60	4114	0	TRP B	130	53.209	86.847	4.127	1.00	87.42
	4115	N	TYR B	131	55.259	86.362	4.940	1.00	97.57
	4116 4117	CA CB	TYR B	131	55.848	86.212	3.621	1.00	97.57
	4117	CG	TYR B TYR B	131 131	57.339 57.881	86.504 86.590	3.647 2.250	1.00	249.42
65	4119	CD1	TYR B	131	57.611	87.707	1.453	1.00 1.00	249.42 249.42
	4120	CE1	TYR B	131	57.982	87.746	0.133	1.00	249.42
	4121	CD2	TYR B	131	58.554	85.514	1.676	1.00	249.42
	4122	CE2	TYR B	131	58.929	85.544	0.355	1.00	249.42
70	4123 4124	CZ OH	TYR B TYP B	131 131	58.628 58.902	86.660 86.675	-0.404 1.706	1.00	249.42
, 5	7167	U (1	Tica D	131	58.902	86.675	-1.726	1.00	249.42

	4125	C	TYR B	131	55.619	04.761	2004	4.00	
	4126	ŏ	TYR B		54.661	84.751 84.439	3.231 2.509	1.00	97.57
	4127	Ň	GLU B	132	56.517	83.862	3.669	1.00 1.00	97.57
	4128	CA	GLU B	132	56.333	82.428	3.432	1.00	249.33 249.33
5	4129	· CB	GLU B	132	57.528	81.602	3.941	1.00	249.46
	4130	CG	GLU B	132	58.788	81.623	3.066	1.00	249.46
	4131	CD	GLU B	132	59.162	80.239	2.532	1.00	249.46
	4132	OE1	GLU B	132	58.693	79.231	3.102	1.00	249.46
10	4133	OE2	GLU B		59.935	80.161	1.551	1.00	249.46
10	4134	C	GLU B	132	55.158	82.276	4.384	1.00	249.33
	4135 4136	0 N	GLU B	132	55.259	82.685	5.543	1.00	249.33
	4137	CA	ASN B	133 133	54.047 52.884	81.711 81.642	3.924 4.798	1.00	134.43
	4138	CB	ASN B		51.649	81.176	4.033	1.00 1.00	134.43 135.42
15	4139	ČĞ	ASN B	133	51.534	79.690	3.981	1.00	135.42
	4140	OD1	ASN B		52.489	78.995	3.617	1.00	135.42
	4141	ND2	ASN B	133	50.358	79.176	4.337	1.00	135.42
	4142	С	ASN B		53.019	80.848	6.080	1.00	134.43
20	4143	0	ASN B		54.026	80.185	6.338	1.00	134.43
20	4144	N	HIS B		51.962	80.932	6.875	1.00	135.01
	4145 4146	CA CB	HIS B		51.905	80.302	8.174	1.00	135.01
	4147	CG	HIS B		52.150 52.262	81.381 80.865	9.224	1.00	225.09
	4148	CD2	HIS B		51.493	81.086	10.622 11.714	1.00 1.00	225.09
25	4149	ND1	HIS B		53.283	80.038	11.032	1.00	225.09 225.09
	4150	CE1	HIS B		53.140	79.772	12.320	1.00	225.09
	4151	NE2	HIS B	134	52.063	80.396	12.756	1.00	225.09
	4152	С	HIS B	134	50.531	79.673	8.355	1.00	135.01
20	4153	0	HIS B	134	49.789	79.494	7.385	1.00	135.01
30	4154	N	ASN B	135	50.197	79.346	9.601	1.00	105.44
	4155 4156	CA CB	ASN B	135	48.928	78.730	9.922	1.00	105.44
	4157	CG	ASN B	135 135	49.090	77.209 76.600	10.001	1.00	235.21
	4158	OD1	ASN B	135	49.415 48.779	76.600 76.948	8.653 7.657	1.00 1.00	235.21
35	4159	ND2	ASN B	135	50.383	75.689	8.604	1.00	235.21 235.21
	4160	C	ASN B	135	48.399	79.280	11.223	1.00	105.44
	4161	0	ASN B	135	48.611	78.700	12.279	1.00	105.44
	4162	N	ILE B	136	47.718	80.417	11.134	1.00	66.02
40	4163	CA	ILE B	136	47.123	81.076	12.304	1.00	66.02
40	4164	CB CG2	ILE B	136	46.015	82.066	11.860	1.00	141.15
	4165 4166	CG1	ILE B	136 136	45.045 45.283	81.385	10.926	1.00	141.15
	4167	CD1	ILE B	136	44.290	82.620 83.673	13.068 12.695	1.00 1.00	141.15
	4168	Č.	ILE B	136	46.555	80.069	13.307	1.00	141.15 66.02
45	4169	Ö	ILE B	136	45.602	79.339	13.022	1.00	66.02
	4170	N	SER B	137	47.160	80.045	14.486	1.00	95.21
	4171	CA	SER B	137	46.768	79,114	15.538	1.00	95.21
	4172	CB	SER B	137	47.968	78.233	15.897	1.00	97.51
50	4173	OG	SER B	137	47.742	77.531	17.105	1.00	97.51
50	4174 4175	C O	SER B	137 137	46.218	79.776	16.807	1.00	95.21
	4176	Ň	ILE B	138	46.625 45.298	80.869 79.095	17.185	1.00	95.21
	4177	CA	ILE B	138	44.698	79.625	17.472 18.688	1.00 1.00	236.44
	4178	CB	ILE B	138	43.295	80.153	18.420	1.00	236.44 113.67
55	4179	CG?	ILE B	138	42.601	80.445	19.737	1.00	113.67
	4180	CG1	ILE B	138	43.363	81.397	17.533	1.00	113.67
	4181	CD1	ILE B	138	42.021	81.787	16.948	1.00	113.67
	4182	Ç	ILE B	138	44.580	78.558	19.761	1.00	236.44
60	4183 4184	0 N	ILE B	138	43.936	77.531	19.555	1.00	236.44
00	4185	CA	THR B	139 139	45.180	78.816	20.915	1.00	117.60
	4186	CB	THR B	139	45.131 46.259	77.865 78.143	22.018	1.00	117.60
	4187	OG1	THR B	139	46.227	79.521	23.020 23.406	1.00 1.00	212.12
	4188	CG2	THR B	139	47.609	77.830	22.390	1.00	212.12 212.12
65	4189	С	THR B	139	43.780	77.942	22.733	1.00	117.60
	4190	0	THR B	139	42.898	77.092	22.541	1.00	117.60
	4191	N	ASN B	140	43.633	78.960	23.573	1.00	147.27
	4192	CA CB	ASN B	140	42.396	79.189	24.308	1.00	147.27
70	4193 4194	CB CG	ASN B	140	42.685	79.890	25.631	1.00	247.00
	7134	~	VOIA D	140	41.426	80.263	26.369	1.00	247.00

	4195	OD1	ASN B	140		80.833	25.789	1.00	247.00
	4196	ND2	ASN B	140	41.395	79.951	27.658	1.00	247.00
	4197	C .	ASN B	140	41.572	80.103	23.421	1.00	147.27
5	4198 4199	O .	ASN B	140	42.004	81.206	23.092	1.00	147.27
,	4200	CA	ALA B ALA B	141	40.383	79.652	23.048	1.00	102.95
	4201	CB	ALA B	141 141	39.537	80.432	22.163	1.00	102.95
	4202	Č	ALA B	141	38.862 38.493	79.519	21.162	1.00	101.29
	4203	ŏ	ALA B	141	37.722	81.273	22.850	1.00	102.95
10	4204	Ň	THR B	142	38.458	80.782 82.546	23.680	1.00	102.95
••	4205	ČA	THR B	142	37.495	83.478	22.474	1.00	139.44
	4206	CB	THR B	142	38.055	84.903	23.021 22.959	1.00	139.44
	4207	OG1	THR B	142	39.366	84.918	23.544	1.00 1.00	140.37
	4208	CG2	THR B	142	37.166	85.858	23.725	1.00	140.37
15	4209	C	THR B	142	36.220	83.361	22.184	1.00	140.37
	4210	Ö	THR B	142	36.216	82.675	21.160	1.00	139.44 139.44
	4211	N	VAL B	143	35.132	83.988	22.623	1.00	168.09
	4212	CA	VAL B	143	33.884	83.922	21.866	1.00	168.09
	4213	υB	VAL B	143	32.633	84.134	22.755	1.00	243.26
20	4214	CG1	VAL B	143	32.616	85.552	23.305	1.00	243.26
	4215	CG2	VAL B	143	31.366	83.867	21.946	1.00	243.26
	4216	С	VAL B	143	33.925	85.029	20.834	1.00	168.09
	4217	0	VAL B	143	33.150	85.035	19.878	1.00	168.09
25	4218	N	GLU B	144	34.839	85.971	21.035	1.00	126.58
25	4219	CA	GLU B	144	34.975	87.081	20.108	1.00	126.58
	4220	СВ	GLU B	144	35.750	88.229	20.751	1.00	249.26
	4221	CG	GLU B	144	35.040	88.850	21.940	1.00	249.26
	4222	CD	GLU B	144	35.771	88.603	23.243	1.00	249.26
30	4223	OE1	GLU B	144	36.942	89.024	23.353	1.00	249.26
30	4224	OE2	GLU B	144	35.181	87.989	24.157	1.00	249.26
	4225	C	GLU B	144	35.673	86.623	18.840	1.00	126.58
	4226 4227	0	GLU B	144	35.633	87.305	17.826	1.00	126.58
	4228	N CA	ASP B ASP B	145	36.307	85.457	18.903	1.00	80.30
35	4229	CB	ASP B ASP B	145 145	36.997	84.893	17.752	1.00	80.30
-	4230	CG	ASP B	145	37.911 39.132	83.753	18.189	1.00	204.44
	4231	OD1	ASP B	145	39.896	84.250 85.030	18.918	1.00	204,44
	4232	OD2	ASP B	145	39.326	83.869	18.310 20.092	1.00	204.44
	4233	C	ASP B	145	36.026	84.395	16.699	1.00 1.00	204.44
40	4234	ō	ASP B	145	36.421	84.133	15.569	1.00	80.30
	4235	N	SER B	146	34.755	84.263	17.062	1.00	80.30 110.67
	4236	CA	SER B	146	33.761	83.800	16.108	1.00	110.67
	4237	CB	SER B	146	32.421	83.569	16.815	1.00	166.23
	4238	OG	SER B	146	32.547	82.573	17.814	1.00	166.23
45	4239	С	SER B	146	33.646	84.870	15.022	1.00	110.67
	4240	0	SER B	146	33.736	86.063	15.302	1.00	110.67
	4241	N	GLY B	147	33.487	84.436	13.778	1.00	85.62
	4242	CA	GLY B	147	33.375	85.365	12.670	1.00	85.62
50	4243	C	GLY B	147	33.473	84.63 5	11.353	1.00	85.62
50	4244 4045	0	GLY B	147	33.311	83.417	11.301	1.00	85.62
	4245 4246	N CA	THR B	148	33.737	85.372	10.279	1.00	63.43
	404=		THR B	148	33.851	84.756	8.952	1.00	63.43
	424 <i>7</i> 4248	CB OG1	THR B	148	32.729	85.244	7.6 11	1.00	111.42
55	4249	CG2	THR B THR I	148 148	33.253 31.609	86.223	7.103	1.00	111.42
-	4250	C	THR B	148		85.879	8.767	1.00	111.42
	4251	ŏ	THA B	148	35.227 35.568	85.092 86.244	8.397	1.00	63.43
	4252	Ň	TYR B	149	36.024	84.069	8.176 8.183	1.00	63.43
	4253	CA	TYR B	149	37.366	84.273	7.705	1.00	61.50
60	4254	CB	TYR B	149	38.298	83.380	8.514	1.00	61.50
	4255	CG	TYR B	149	38.353	83.629	10.007	1.00 1.00	61.70
	4256	CD1	TYR B	149	37.273	83.361	10.839	1.00	61.70
	4257	CE1	TYR B	149	37.373	83.572	12.217	1.00	61.70 61.70
~~	4258	CD2	TYR B	149	39.514	84.106	10.587	1.00	61.70
65	4259	CE2	TYR B	149	39.626	84.317	11.939	1.00	61.70
	4260	CZ	TYR B	149	38.571	84.060	12.757	1.00	61.70
	4261	ŎН	TYR B	149	38.744	84.327	14.104	1.00	61.70
	4262	C	TYR B	149	37.540	83.934	6.223	1.00	61.50
70	4263	0	TYR B	149	36.666	83.307	5.605	1.00	61.50
70	4264	N	TYR B	150	38.674	84.372 _.	5.669	1.00	57.66

	4265	CA	TYR B	150	39.090	84.071	4.302	1.00	57.66
	4266 4267	CB CG	TYR B	150	38.189	84.760	3.264	1.00	101.41
	4268	CD1	TYR B TYR B	150 150	38.386 39.493	86.234 86.704	3.018	1.00	101.41
5	4269	CE1	TYR B	150	39.653	86.704 88.065	2.338 2.074	1.00 1.00	101.41
	4270	CD2	TYR B	150	37.435	87.160	3.428	1.00	101.41
	4271	CE2	TYR B	150	37.582	88.520	3.163	1.00	101.41 101.41
	4272	CZ	TYR B	150	38.693	88.967	2.489	1.00	101.41
10	4273	ОН	TYR B	150	38.855	90.316	2.245	1.00	101.41
10	4274	C	TYR B	150	40.539	84.536	4.251	1.00	57.66
	4275 4276	0 N	TYR B CYS B	150	40.952	85.331	5.109	1.00	57.66
	4277	CA CA	CYS B	151 151	41.340 42.736	84.020 84.458	3.318	1.00	78.79
	4278	Č	CYS B	151	43.124	84.856	3.227 1.804	1.00	78.79
15	4279	Ö	CYS B	151	42.464	84.461	0.849	1.00 1.00	78.79 78.79
	4280	CB	CYS B	151	43.680	83.369	3.736	1.00	103.97
	4281	SG	CYS B	151	43.510	81.730	2.951	1.00	103.97
	4282	N	THR B	152	44.174	85.668	1.673	1.00	109.05
20	4283	CA	THR B	152	44.663	86.107	0.370	1.00	109.05
20	4284 4285	CB OG1	THR B	152	44.524	87.630	0.206	1.00	169.15
	4286	CG2	THR B	152 152	45.394 43.097	88.296 88.056	1.133	1.00	169.15
	4287	C	THR B	152	46.139	85.728	0.475 0.2 9 7	1.00 1.00	169.15
	4288	Ö	THR B	152	46.839	85.740	1.317	1.00	109.05 109.05
25	4289	N	GLY B	153	46.611	85.381	-0.898	1.00	135.93
	4290	CA	GLY B	153	48.007	85.000	-1.054	1.00	135.93
	4291	Ç	GLY B	153	48.447	85.023	-2.501	1.00	135.93
	4292	0	GLY B	153	47.618	85.025	-3.404	1.00	135.93
30	4293 4294	N CA	LYS B	154	49.751	85.038	-2.734	1.00	88.42
50	4295	CB	LYS B LYS B	154 154	50.252	85.068	-4.096	1.00	88.42
	4296	CG	LYS B	154	51.392 51.920	86.090 86.317	-4.216 -5.630	1.00	187.09
	4297	CD	LYS B	154	53.003	87.393	-5.619	1.00 1.00	187.09
	4298	CE	LYS B	154	53.634	87.579	-6.975	1.00	187.09 187.09
35	4299	NZ	LYS B	154	54.766	88.490	-6.839	1.00	187.09
	4300	C	LYS B	154	50.744	83.673	-4.404	1.00	88.42
	4301	Ö	LYS B	154	51.450	83.057	-3.592	1.00	88.42
	4302 4303	N CA	VAL B VAL B	155	50.332	83.166	-5.561	1.00	135.91
40	4304	CB	VAL B VAL B	155 155	50.742 49.550	81.845	-6.018	1.00	135.91
	4305	CG1	VAL B	155	50.030	80.923 79.574	-6.254 -6.748	1.00	118.28
	4306	CG2	VAL B	155	48.773	80.767	-4.968	1.00 1.00	118.28 118.28
	4307	С	VAL B	155	51.459	82.067	-7.332	1.00	135.91
45	4308	0	VAL B	155	50.938	82.731	-8.237	1.00	135.91
45	4309	N	TRP B	156	52. 65 5	81.505	-7.433	1.00	121.66
	4310 4311	CA	TRP B	156	53.453	81.702	-8.624	1.00	121.66
	4312	CB CG	TRP B	156	52.679	81.359	-9.884	1.00	200.98
	4313	CD2	TRP B	156 156	52.385 53.333	79.963 78.905	-9.953 0.004	1.00	200.98
50	4314	CE2	TRP B	156	52.609	77.699	-9.901 -9.939	1.00 1.00	200.98
	4315	CE3	TRP B	156	54.730	78.860	-9.823	1.00	200.98 200.98
	4316	CD1	TRP B	156	51.160	79.393	-10.027	1.00	200.98
	4317	NE1	TRP B	156	51.283	78.024	-10.013	1.00	200.98
55	4318	CZ2	TRP B	156	53.232	76.454	-9.905	1.00	200.98
23	4319	CZ3	TRP B	156	55.352	77.622	-9.790	1.00	200.98
	4320 4321	CH2 C	TRP B	156	54.59 ₅	76.432	-9.834	1.00	200.98
	4322	ŏ	TRP B	156 156	53.739	83.168	-8.671	1.00	121.66
	4323	Ň	GLN B	157	54.677 52.883	83.647 83.878	-8.029 0.403	1.00	121.66
60	4324	CA	GLN B	157	53.057	85.297	-9.403 -9.568	1.00 1.00	111.84
	4325	CB	GLN B	157	53.912	85.525	-10.808	1.00	111.84 249.48
	4326	CG	GLN B	157	55.364	85.155	-10.531	1.00	249.48
	4327	CD	GLN B	157	55.818	85.806	-9.260	1.00	249.48
65	4328	OE1	GLN B	157	55.599	86.983	-9.081	1.00	249.48
O)	4329 4330	NE2	GLN B	157	56.437	85.047	-8.360	1.00	249.48
	4330	C	GLN B GLN B	157	51.781	86.092	-9.614	1.00	111.84
	4332	Ň	LEU B	157 158	51.785 50.688	87.265 85.447	-9.988	1.00	111.84
	4333	CA	LEU B	158	49.392	85.447 86.104	-9.217 -9.195	1.00	140.68
70	4334	CB	LEU B	158	48.463	85.512	-9.195 -10.253	1.00 1.00	140.68 225.85
							- 10.200	1.00	حدی.55

	4335	~	LEU B	450					
	4335	CG CD1	LEV B	158 ⁻ 158	48.673 47.296	85.926 86.093	-11.710 -12.325	1.00 1.00	225.85
	4337	CD2	LEU B	158	49.447	87.239	-11.827	1.00	225.85 225.85
5	4338	Ç	LEU B	158	48.724	86.035	-7.829	1.00	140.68
2	4339 4340	0 N	LEU B ASP B	158	48.980	85.125 07.017	-7.039	1.00	140.68
	4341	CA	ASP B	159 159	47.870 47.162	87.017 87.101	-7.560 -6.291	1.00 1.00	142.12 142.12
	4342	CB	ASP B	159	46.879	88.574	-5.943	1.00	249.27
10	4343	CG	ASP B	159	48.138	89.443	-5.949	1.00	249.27
10	4344 4345	OD1 OD2	ASP B ASP B	159 159	49.066	89.181	-5.152	1.00	249.27
	4346	C	ASP B	159	48.194 45.846	90.399 86.325	-6.754 -6.363	1.00 1.00	249.27
	4347	0	ASP B	159	45.204	86.280	-7.414	1.00	142.12 142.12
15	4348	N	TYR B	160	45.456	85.711	-5.244	1.00	173.61
13	4349 4350	CA CB	TYR B TYR B	160 160	44. 2 09 44.442	84.946 83.463	-5.164 5.420	1.00	173.61
	4351	CG	TYR B	160	45.173	83.176	-5.430 -6.709	1.00 1.00	249.32 249.32
	4352	CD1	TYR B	160	46.561	83.098	-6.731	1.00	249.32
20	4353	CE1	TYR B	160	47.246	82.846	-7.908	1.00	249.32
20	4354 4355	CD2 CE2	TYR B TYR B	160 160	44.481 45.155	82.995 82.744	-7.903 -9.091	1.00	249.32
	4356	CZ	TYR B	160	46.540	82.671	-9.085	1.00 1.00	249.32 249.32
	4357	ÓН	TYR B	160	47.221	82.428	-10.254	1.00	249.32
25	4358	C	TYR B	160	43.517	85.072	-3.818	1.00	173.61
23	4359 4360	O N	TYR B GLU B	160 161	44.155 42.194	85.185 85.014	-2.768 -3.871	1.00	173.61
	4361	CA	GLU B	161	41.341	85.130	-3.67 i -2.695	1.00 1.00	90.61 90.61
	4362	СВ	GLU B	161	40.333	86.257	-2.926	1.00	219.32
30	4363 4364	CG CD	GLU B	161	39.312	86.469	-1.834	1.00	219.32
50	4365	OE1	GLU B	161 161	38.626 37.530	87.808 87.986	-1.980 -1.409	1.00 1.00	219.32
	4366	OE2	GLU B	161	39.197	88.688	-2.663	1.00	219.32 219.32
	4367	C	GLU B	161	40.634	83.792	-2.513	1.00	90.61
35	4368 4369	0 N	GLU B SER B	161 162	40.215 40.522	83,179	-3.486	1.00	90.61
-	4370	ČA	SER B	162	39.884	83.335 82.057	-1.270 -0.957	1.00 1.00	91.35 91.35
	4371	СВ	SER B	162	40.575	81.414	0.251	1.00	56.32
	4372	OG .	SER B	162	40.507	82.266	1.391	1.00	56.32
40	4373 4374	C O	SER B SER B	162 162	38.401 37.909	82.220 83.344	-0.664 -0.522	1.00	91.35
	4375	Ň	GLU B	163	37.690	81.097	-0.522 -0.574	1.00 1.00	91.35 79.84
	4376	CA	GLU B	163	36.253	81.114	-0.287	1.00	79.84
	4377 4378	CB CG	GLU B GLU B	163	35.639	79.737	-0.529	1.00	200.03
45	4379	CD	GLU B	163 163	35.475 34.355	79.360 80.127	-1.993 -2.674	1.00 1.00	200.03 200.03
	4380	OE1	GLU B	163	33.206	80.054	-2.187	1.00	200.03
	4381	OE2	GLU B	163	34.621	80.795	-3.698	1.00	200.03
	4382 4383	C O	GLU B	163 163	36.094 36.886	81.500 81.075	1.169	1.00	79.84
50	4384	Ň	PRO B	164	35.068	81.075 82.315	1.996 1.508	1.00 1.00	79.84 60.77
	4385	CD	PRO B	164	34.003	82.898	0.682	1.00	73.97
	4386	CA	PRO B	164	34.904	82.700	2.920	1.00	60.77
	4387 4388	CB CG	PRO B PRO B	164 164	33.877 33.008	83.829 83.388	2.847	1.00	73.97
55	4389	Č	PRO B	164	34.431	81.530	1.730 3.744	1.00 1.00	73.97 60.77
	4390	0	PRO B	164	33.842	80.588	3.223	1.00	6°.77
	4391 4392	N CA	LEU B	165	34.700	81.568	5.035	1.00	63.41
	4393	CA CB	LEU B LEU B	165 165	34.288 35.440	80.472 79.499	5.889	1.00	63.41
60	4394	CG	LEU B	165	35.185	78.450	6.070 7.138	1.00 1.00	68.59 68.59
	4395	CD1	LEU B	165	33.824	77.858	6.851	1.00	68.59
	4396 4397	CD2	LEU B	165	38.264	77.380	7.140	1.00	68.59
	4398	C	LEU B LEU B	165 165	33.847 34.613	80.963 81.635	7.250 7.953	1.00	63.41
65	4399	N	ASN B	166	32.623	80.613	7.953 7.628	1.00 1.00	63.41 64.97
	4400	CA	'ASN B	166	32.078	81.041	8.911	1.00	64.97
	4401 4402	CB CG	ASN B ASN B	166	30.556	81.011	8.900	1.00	96.05
	4403	OD1	ASN B	166 166	29.945 30.504	82.338 83.403	8.491 8.737	1.00	96.05
70	4404	ND2	ASN B	166	28.773	82.270	7.884	1.00 1.00	96.05 96.05

	4405	С	ASN B	166	32.556	80.174	10.040	1.00	24.0-
	4406	Ó	ASN B	166	32.754	78.988	9.860	1.00	64.97
	4407	Ν .	ILE B	167	32.720	80.766	11.213	1.00	64.97 77.41
_	4408	CA	ILE B	167	33.183	80.034	12.375	1.00	77.41
5	4409	CB	ILE B	167	34.653	80.263	12.591	1.00	59.98
	4410	CG2	ILE B	167	35.050	79.859	13.985	1.00	59.98
	4411 4412	CG1 CD1	ILE B	167	35.434	79.484	11.546	1.00	59.98
	4413	C	ILE B	167 167	36.942 32.467	79.537	11.784	1.00	59.98
10	4414	ŏ	ILE B	167	32.375	80.488 81.676	13.622 13.896	1.00	77.41
	4415	Ň	THR B	168	31.972	79.548	14.405	1.00 1.00	77.41
	4416	CA	THR B	168	31.283	79.938	15.610	1.00	104.04 104.04
	4417	СВ	THR B	168	29.817	79.572	15.536	1.00	107.45
15	4418	OG1	THR B	168	29.239	80.179	14.374	1.00	107.45
15	4419	CG2	THR B	168	29.096	80.067	16.766	1.00	107.45
	4420	C	THR B	168	31.888	79.326	16.850	1.00	104.04
	4421 4422	0 N	THR B	168	32.254	78.155	16.886	1.00	104.04
	4423	CA	VAL B	169 169	32.012 32.544	80.155	17.867	1.00	108.46
20	4424	CB	VAL B	169	33.748	79.737 80.618	19.146	1.00	108.46
	4425	CG1	VAL B	169	33.974	80.539	19.563 21.049	1.00 1.00	68.82
	4426	CG2	VAL B	169	34.981	80.174	18.834	1.00	68.82 68.82
•	4427	С	VAL B	169	31.394	79.942	20.129	1.00	108.46
~~	4428	0	VAL B	169	31.047	81.082	20.455	1.00	108.46
25	4429	N	ILE B	170	30.790	78.844	20.579	1.00	128.18
	4430	CA	ILE B	170	29.679	78.917	21.525	1.00	128.18
	4431	CB	ILE B	170	28.680	77.760	21.285	1.00	141.23
	4432 4433	CG2	ILE B	170	28.276	77.749	19.833	1.00	141.23
30	4434	CG1 CD1	ILE B	170	29.321	76.414	21.631	1.00	141.23
50	4435	C	ILE B	170 170	28.423 30.228	75.218 79.954	21.463	1.00	141.23
	4436	ŏ	ILE B	170	31.426	78.854 78.679	22.946 23.142	1.00	128.18
	4437	Ň	LYS B	171	29.365	79.005	23.941	1.00 1.00	128.18
	4438	CA	LYS B	171	29.816	78.956	25.328	1.00	164.76 164.76
35	4439	CB	LYS B	171	29.779	80.358	25.929	1.00	211.84
	4440	CG	LYS B	171	28.416	81.020	25.858	1.00	211.84
	4441	CD	LYS B	171	28.536	82.537	25.911	1.00	211.84
	4442 4443	CE NZ	LYS B	171	29.207	83.011	27.190	1.00	211.84
40	4444	C	LYS B	171 171	29.341	84.494	27.217	1.00	211.84
	4445	ŏ	LYS B	171	28.987 29.329	77.998 77.724	26.180 27.330	1.00	164.76
	4446	C1	NAG B	221	47.345	59.956	-1.693	1.00 1.00	164.76
	4447	C2	NAG B	221	48.521	60.923	-1.796	1.00	249.77 249.77
	4448	N2	NAG B	221	48.022	62.275	-1.936	1.00	249.77
45	4449	C 7	NAG B	221	48.763	63.299	-1.535	1.00	249.77
	4450	07	NAG B	221	49.873	63.160	-1.022	1.00	249.77
	4451 4452	C8	NAG B	221	48.181	64.690	-1.724	1.00	249.77
	4453	C3 O3	NAG B	221	49.387	60.591	-3.002	1.00	249.77
50	4454	C4	NAG B	221 221	50. 56 0 49. 78 3	61.387	-2.974	1.00	249.77
	4455	04	NAG B	221	50.388	59.115 58.867	-3.044 -4.330	1.00	249.77
	4456	C5	NAG B	221	48.535	58.221	-4.330 -2.850	1.00 1.00	249.77 249.77
	4457	O 5	NAG B	221	47.825	58.605	-1.651	1.00	249.77 249.77
<i>e e</i>	4458	C6	NAG B	221	48.869	56.745	-2.696	1.00	249.77
55	4459	Q6	NAG B	221	49.689	56.518	-1.557	1.00	249.77
	4460	C1	NAG B	222	51.148	57.718	-4.505	1.00	249.77
	4461 4462	C2 N2	NAG B	222	52.440	58.058	-5.267	1.00	249.77
	4463	C7	NAG B	222 222	53.222	59.027	-4.521	1.00	249.77
60	4464	O7	NAG B	222	54.445 54.970	58.717 57.633	-4.103	1.00	249.77
	4465	C8	NAG B	222	55.199	57.622 59.786	-4.314 -3.332	1.00 1.00	249.77
	4466	C3	NAG B	222	52.103	58.614	-6.661	1.00	249.77 249.77
	4467	O3	NAG B	222	53.301	58.775	-7.409	1.00	249.77
45	4468	C4	NAG B	222	51.148	57.668	-7.412	1.00	249.77
65	4469	04	NAG B	222	50.712	58.282	-8.619	1.00	249.77
	4470	C5	NAG B	222	49.930	57.333	-6.541	1.00	249.77
	4471 4472	O5	NAG B	222	50.362	56.787	-5.270	1.00	249.77
	4473	C6 O6	NAG B	222 222	49.003	56.316	-7.180	1.00	249.77
70	4474	C1	NAG B NAG B	242	47.646 26.466	56.720 62.870	-7.068	1.00	249.77
	•		TO DAY	-74	26.466	62.870	-0.923	1.00	89.47

	4475	C2	NAG B	242 -	26.972	62.476	-2.293	1.00	89.47
	4476	N2	NAG B	242	27.712	61.243	-2.203	1.00	89.47
	4477	C7	NAG B	242	27.358	60.216	-2.956	1.00	89.47
5	4478	07	NAG B	242	26.416	60.270	-3.732	1.00	89.47
J	4479 4480	C8 C3	NAG B	242	28.159	58.938	-2.829	1.00	89.47
	4481	∝ ⊙3	NAG B NAG B	242 242	27.882 28.253	63.561 53 .234	-2.855	1.00	89.47
	4482	C4	NAG B	242	27.180	64.901	-4.180 -2.854	1.00 1.00	89.47
	4483	04	NAG B	242	28.116	65.947	-3.186	1.00	89.47 89.47
10	4484	C5	NAG B	242	26.567	65.197	-1.493	1.00	89.47
	4485	Q5	NAG B	242	25.753	64.083	-1.046	1.00	89.47
	4486	C6	NAG B	242	25.657	66.413	-1.634	1.00	89.47
	4487 4488	O6 C1	NAG B NAG B	242 243	25.965	67.439).691	1.00	89.47
15	4489	C2	NAG B	243	27.860 28.444	66.616 68.031	363 -4.311	1.00 1.00	124.06
	4490	N2	NAG B	243	27.812	68.814	-3.263	1.00	124.06 124.06
	4491	C7	NAG B	243	28.560	69.543	-2.441	1.00	124.06
	4492	07	NAG B	243	29.786	69.568	-2.502	1.00	124.06
20	4493	C8	NAG B	243	27.853	70.353	-1.378	1.00	124.06
20	4494 4495	C3 O3	NAG B	243	28.214	63.724	-5.658	1.00	124.06
	4496	Ω 24	NAG B NAG B	243 243	28.825 28.765	70.012 67.860	-5.653 -6.816	1.00	124.06
	4497	04	NAG B	243	28.392	68.459	-8.089	1.00 1.00	124.06
	4498	C5	NAG B	243	28.162	6o.455	-6.717	1.00	124.06 124.06
25	4499	O5	NAG B	243	28.449	65.870	-5.432	1.00	124.06
	4500	C6	NAG B	243	28.638	65.499	-7.762	1.00	124.06
	4501	O6	NAG B	243	30.003	65.214	-7.571	1.00	124.06
	4502 4503	C1 C2	MAN B MAN B	244	29.308 30.527	68.650	-9.080	1.00	182.20
30	4504	02	MAN B	244 244	30.527 31.636	69.553 68.751	-8.800 -8.489	1.00 1.00	182.20
	4505	C3	MAN B	244	30.736	70.260	-10.177	1.00	182.20 182.20
	4506	03	MAN B	244	31.834	71.153	-10.165	1.00	182.20
	4507	<u>C4</u>	MAN B	244	30.850	69. 26 4	-11.367	1.00	182.20
35	4508	O4	MAN B	244	31.059	69.973	-12.588	1.00	182.20
33	4509 4510	C5 O5	MAN B MAN B	244 244	29.519	68.480	-11.433	1.00	182.20
	4511	C6	MAN B	244 244	29.290 29.376	67.732 67.561	-10.210 -12.650	1.00 1.00	182.20
	4512	06	MAN B	244	30.030	66.327	-12.454	1.00	182.20 182.20
40	4513	C1	NAG B	250	42.367	49.115	8.367	1.00	249.70
40	4514	C2 .	NAG B	250	43.729	49.074	9.087	1.00	249.70
	4515	N2	NAG B	250	43.544	49.049	10.526	1.00	249.70
	4516 4517	C7 O7	NAG B NAG B	250	43.853	47.960	11.227	1.00	249.70
	4518	C8	NAG B	250 250	44.295 43.632	46.930 48.021	10.709 12.734	1.00 1.00	249.70
45	4519	C3	NAG B	250	44.545	50.311	8.692	1.00	249.70 249.70
	4520	O3	NAG B	250	45.842	50.245	9.269	1.00	249.70
	4521	C4	NAG B	250	44.660	50.407	7.167	1.00	249.70
	4522 4523	04 05	NAG B	250	45.304	51.625	6.813	1.00	249.70
50	4523 4524	C5 O5	NAG B NAG B	250 250	43.262 42.562	50.349	6.521	1.00	249.70
-	4525	C6	NAG B	250	43.315	49.158 50.314	6.946 5.003	1.00 1.00	249.70
	4526	06	NAG B	250	42.060	49.940	4.449	1.00	249.70 249.70
	4527	C1	NAG B	274	20.954	54.260	22.053	1.00	246.89
55	4528	C2	NAG B	274	20.822	55.380	23.099	1.00	246.89
55	4529	N2	NAG B	274	21.918	55.314	24.050	1.00	246 90
	4530 4531	C7 O7	NAG B NAG B	274	22.298	56.407	24.706	1.00	246.89
	4532	C8	NAG B	274 274	21.767 23.446	57.506 56.263	24.541 25.690	1.00 1.00	246.89
	4533	Č	NAG B	274	19.484	55.246	23.844	1.00	246.89 246.89
60	4534	O 3	NAG B	274	19.302	56.360	24.707	1.00	246.89
	4535	C4	NAG B	274	18.314	55.163	22.856	1.00	246.89
	4536 4537	04 C5	NAG B	274	17.111	54.887	23.563	1.00	246.89
	4537 4538	C5 O5	NAG B NAG B	274 274	18.576	54.059 54.201	21.820	1.00	246.89
65	4539	C6	NAG B	274 274	19.837 17.507	54.291 53.987	21.151 20.743	1.00 1.00	246.89
	4540	06	NAG B	274	17.896	53.120	19.688	1.00	246.89 246.89
	4541	C1	NAG B	335	50.085	74.386	8.041	1.00	247.49
	4542	C2	NAG B	335	50.430	73.230	9.006	1.00	247.49
70	4543 4544	N2	NAG B	335	50.451	73.760	10.357	1.00	247.49
70	4544	C7	NAG B	33 5	49.583	73.330	11.267	1.00	247.49

	4545 4546 4547	O7 C8	NAG B NAG B	335 335	48.734 49.680	72.471 73.947	11.036 12.649	1.00 1.00	247.49 247.49
	4548	C3 O3	NAG B NAG B	335 335	51.781	72.552	8.725	1.00	247.49
5	4549	Č	NAG B	335	51.808 52.016	71.282 72.369	9.359	1.00	247.49
	4550	04	NAG B	335	53.304	71.813	7.231 7.004	1.00	247.49
	4551	C5	NAG B	335	51.906	73.729	6.561	1.00 1.00	247.49
	4552	O5	NAG B	335	50.550	74.212	6.679	1.00	247.49 247.49
10	4553	C6	NAG B	335	52.229	73.654	5.078	1.00	247.49
10	4554 4555	O6	NAG B	335	53.343	74.471	4.748	1.00	247.49
	4556	C1 C2	NAG B NAG B	340 340	41.414	81.009	28.648	1.00	249.67
	4557	N2	NAG B	340	40.114 38.971	80.981 81.033	29.434 28.539	1.00	249.67
	4558	C7	NAG B	340	37.997	80.133	28.666	1.00 1.00	249.67
15	4559	07	NAG B	340	38.012	79.245	29.526	1.00	249.67 249.67
	4560	C8	NAG B	340	36.831	80.226	27.702	1.00	249.67
	4561 4562	C3	NAG B	340	40.092	82.143	30.420	1.00	249.67
	4563	O3 C4	NAG B NAG B	340 340	38.904	82.071	31.207	1.00	249.67
20	4564	04	NAG B	340	41.329 41.393	82.067 83.255	31.330	1.00	249.67
	4565	C5	NAG B	340	42.643	81.894	32.105 30.520	1.00 1.00	249.67
	4566	O5	NAG B	340	42.519	80.841	29.539	1.00	249.67 249.67
	4567	C6	NAG B	340	43.832	81.515	31.388	1.00	249.67
25	4568	06	NAG B	340	44.745	80.677	30.696	1.00	249.67
23	4569 4570	C1 C2	NAG B NAG B	366 366	28.147	83.475	7.400	1.00	133.05
	4571	N2	NAG B	366	27.352 28.247	83.132 82.591	6.154	1.00	133.05
	4572	C7	NAG B	366	28.452	81.278	5.149 5.075	1.00 1.00	133.05
20	4573	07	NAG B	366	27.909	80.467	5.829	1.00	133.05 133.05
30	4574	C8	NAG B	366	29.408	80.789	3.998	1.00	133.05
	4575 4576	C3 O3	NAG B	366	26.651	84.373	5.618	1.00	133.05
	4577	C4	NAG B NAG B	366 366	25.783 25.842	84.003	4.553	1.00	133.05
	4578	04	NAG B	366	25.403	85.068 86.347	6.713 6.211	1.00	133.05
35	4579	C5	NAG B	366	26.688	85.270	7.986	1.00 1.00	133.05 133.05
	4580	O5	NAG B	366	27.291	84.029	8.400	1.00	133.05
	4581 4582	C6 O6	NAG B	366	25.864	85.757	9.163	1.00	133.05
	4583	C1	NAG B NAG B	366 367	26.677 24.042	85.957 86.610	10.310	1.00	133.05
40	4584	C2	NAG B	367	23.806	88.121	6.284 6.264	1.00 1.00	230.72
	4585	N2	NAG B	367	24.497	88.757	7.369	1.00	230.72 230.72
	4586	C7	NAG B	367	25.574	89.501	7.133	1.00	230.72
	4587 4588	O7 C8	NAG B	367	26.030	89.681	6.002	1.00	230.72
45	4589	cs cs	NAG B ~	367 367	26.251 22.301	90.141	8.334	1.00	230.72
	4590	O3	NAG B	367	22.054	88.392 89.791	6.337 6.274	1.00	230.72
	4591	C4	NAG B	367	21.604	87.688	5.169	1.00 1.00	230.72 230.72
	4592	Q 4	NAG B	367	20.197	87.854	5.276	1.00	230.72
50	4593	C5	NAG B	367	21.956	86.193	5.170	1.00	230.72
50	4594 4595	O5 C6	NAG B NAG B	367	23.395	86.007	5.152	1.00	230.72
	4596	O6	NAG B	367 367	21.396 22.431	85.477 85.064	3.959	1.00	230.72
	4597	СВ	LYS D	4	55.111	67.727	3.078 55.236	1.00	230.72
e e	4598	CG	LYS D	4	54.671	66.297	5-1.972	1.00 1.00	220.56 220.56
55	4599	CD	LYS D	4	54.274	65.601	56.262	1.00	220.56
	4600 4601	CE NZ	LYS D	4	53.817	64.172	56.007	1.00	220.56
	4602	C	LYS D Lys d	4 4	53.427 54.245	63.496	57.274	1.00	220.56
	4603	ŏ	LYS D	4	53.112	68.471 68.293	53.028 53.459	1.00 1.00	175.22
60	4604	N	LYS D	4	55.813	69.908	54.320	1.00	175.22 175.22
	4605	CA	LYS D	4	55.442	68.509	53.968	1.00	175.22
	4606 4607	N CD	PRO D	5	54.485	68.654	51.722	1.00	119.81
	4607 4608	· CD CA	PRO D PRO D	5	55.727	69.166	51.125	1.00	90.67
65	4609	CB	PRO D	5 5	53.397 53.950	68.631 69.490	50.737	1.00	119.81
	4610	ČĠ	PRO D	5	55.400	69.490 69.182	49.602 49.643	1.00 1.00	90.67
	4611	Ç	PRO D	5	53.035	67.215	50.281	1.00	90.67 119.81
	4612	0	PRO D	5	53.836	66.281	50.412	1.00	119.81
70	4613 4614	N CA	LYS D	6	51.824	67.054	49.752	1.00	96.52
	7017	V A	LYS D	6	51.373	65.747	49.285	1.00	96.52

		•							
	4615	CB	LYS D	6	50.549	65.060	50.379	1.00	171.50
	4616	CG	LYS D	6	50.141	63.639	50.041	1.00	171.50
	4617	CD	LYS D	6	49,490	62.929	51.225	1.00	171.50
_	4618	CE	LYS D	6	49.128	61.483	50.860	1.00	
5	4619	NZ	LYS D	6	48.560	60.707	52.003	1.00	171.50
	4620	C	LYS D	6	50.557	65.881	47.994		171.50
	4621	ō	LYS D	6	49.495	66.491	47.981	1.00	96.52
	4622	Ň	VAL D	7	51.072	65.306		1.00	96.52
	4623	CA	VAL D	7	50.422		46.911	1.00	68.94
10	4624	CB	VAL D	7		65.353	45.604	1.00	68.94
10	4625	CG1	VAL D		51.321	64.793	44.498	1.00	87.54
				7	50.661	65.026	43.147	1.00	87.54
	4626	CG2	VAL D	7	52.693	65.408	44.566	1.00	87.54
	4627	Ç	VAL D	7	49.159	64.529	45.521	1.00	68.94
15	4628	0	VAL D	7	49.213	63.311	45.658	1.00	68.94
15	4629	N	SER D	8	48.033	65.178	45.263	1.00	67.77
	4630	CA	SER D	8	46.766	64.465	45.138	1.00	67.77
	4631	CB	SER D	8	45.651	65.209	45.877	1.00	176.15
	4632	OG	SER D	8	45.554	66.551	45.438	1.00	176.15
	4633	С	SER D	8	46.434	64.349	43.651	1.00	67.77
20	4634	0	SER D	8	47.041	65.043	42.834	1.00	67.77
	4635	N	LEU D	9	45.500	63.459	43.304	1.00	116.14
	4636	CA	LEU D	9	45.098	63.252	41.912	1.00	
	4637	СВ	LEU D	9	45.531	61.883	41.396	1.00	116.14
	4638	CG	LEU D	9	47.001	61.491	41.352	1.00	98.23
25	4639	CD1	LEU D	9	47.193	60.359			98.23
	4640	CD2	LEU D	9	47.133	62.671	40.372	1.00	98.23
	4641	C	LEU D	9			40.913	1.00	98.23
	4642	ŏ	LEU D		43.596	63.326	41.770	1.00	116.14
	4643	N		9	42.865	63.094	42.732	1.00	116.14
30	4644	CA	ASN D	10	43.135	63.630	40.560	1.00	87.18
50			ASN D	10	41.699	63.718	40.284	1.00	87.18
	4645	CB	ASN D	10	41.130	65.052	40.768	1.00	123.83
•	4646	CG	ASN D	10	39.625	65.064	40.746	1.00	123.83
	4647	OD1	ASN D	10	38.973	64.342	41.505	1.00	123.83
25	4648	ND2	ASN D	10	39.058	65.867	39.857	1.00	123.83
35	4649	Ç	ASN D	10	41.419	63.561	38.797	1.00	87.18
	4650	0	ASN D	10	41.732	64.453	38.000	1.00	87.18
	4651	N	PRO D	11	40.804	62.432	38.402	1.00	137.25
	4652	CD	PRO D	11	40.609	62.151	36.972	1.00	119.64
40	4653	CA	PRO D	11	40.349	61.301	39.221	1.00	137.25
40	4654	CB	PRO D	11	39.877	60.298	38.167	1.00	119.64
	4655	CG	PRO D	11	39.503	61.164	37.007	1.00	119.64
	4656	C	PRO D	11	41.422	60.689	40.148	1.00	137.25
	4657	0	PRO D	11	42.614	60.926	39.952	1.00	137.25
	4658	N	PRO D	12	41.017	59.899	41.164	1.00	96.57
45	4659	CD	PRO D	12	39.630	59.557	41.534	1.00	
	4660	CA	PRO D	12	41.951	59.269	42.104	1.00	83.9 ·
	4661	CB	PRO D	12	41.041	58.629	43.151	1.00	96.57
	4662	ČĞ	PRO D	12	39.761	59.344			83.91
	4663	č	PRO D				43.011	1.00	83.91
50	4664	ŏ	PRO D	12	42.774	58.205	41.374	1.00	96.57
50	4665	Ň		12	43.874	57.834	41.802	1.00	96.57
	4666	CA	TRP D	13	42.222	57.717	40.268	1.00	86.01
			TRP D	13	42.869	56.675	39.486	1.00	86.01
	4667	CB	THP D	13	42.032	56.366	38.247	1.00	97.24
55	466	CG	TRP D	13	40.601	56.191	38.568	1.00	97.24
22	4669	CD2	TRP D	13	40.049	55.556	39.724	1.00	97.2
	4670	CE2	TRP D	13	38.651	55.664	39.631	1.00	97.24
	4671	CE3	TRP D	13	40.604	54.902	40.836	1.00	97.24
	4672	CD1	TRP D	13	39.546	56.637	37.836	1.00	97.24
	4673	NE1	TRP D	13	38.370	56.330	38.469	1.00	97.24
60	4674	CZ2	TRP D	13	37.795	55.147	40.609	1.00	97.24
	4675	CZ3	TRP D	13	39.753	54.387	41.804	1.00	97.24
	4676	CH2	TRP D	13	38.364	54.515	41.686	1.00	97.24
	4677	С	TRP D	13	44.278	57.041	39.075	1.00	86.01
	4678	Ō	TRP D	13	44.493	58.036	38.401	1.00	86.01
65	4879	Ň	ASN D	14	45.244	56.231	39.488	1.00	79.52
	4680	ĊA	ASN D	14	46.627	56.488	39.122	1.00	
	4681	СВ	ASN D	14	47.534	56.449			79.52
	4682	ČĞ	ASN D	14	47.664	55.067	40.358	1.00	103.31
	4683	OD1	ASN D	14	46.671		40.958	1.00	103.31
70	4684	ND2	ASN D	14	48.895	54.415 54.610	41.283	1.00	103.31
. •		- 100	7011 D	••	70.033	54.618	41.124	1.00	103.31

	4685	С	ASN D	14	47.153	EE EAE	20.024	4.00	
	4686	ŏ	ASN D	14	47.153 48.358	55.545 55.444	38.031 37.825	1.00 1.00	79.52
	4687	N	ARG D	15	46.248	54.842	37.351	1.00	79.52 58.96
5	4688 4689	CA CB	ARG D	15	46.609	53.977	36.231	1.00	58.96
J	4690	CG	ARG D ARG D	15 15	46.413 46.829	52.517 52.131	36.552 37.918	1.00	70.76
	4691	CD	ARG D	15	46.633	50.641	38.077	1.00 1.00	70.76 70.76
	4692	NE	ARG D	15	47.557	49.869	37.263	1.00	70.76
10	4693 4694	CZ NH1	ARG D ARG D	15	47.280	48.660	36.802	1.00	70.76
10	4695	NH2	ARG D	15 15	46.108 48.170	48.121 47.981	37.078 36.079	1.00 1.00	70.76
	4696	С	ARG D	15	45.573	54.375	35.202	1.00	70.76 58.96
	4697	0	ARG D	15	44.384	54.102	35.367	1.00	58.96
15	4698 4699	N CA	ILE D	16 16	46.006 45.052	55.037 55.457	34.144	1.00	65.25
	4700	СВ	ILE D	16	44.928	56.967	33.146 33.117	1.00 1.00	65.25 107.28
	4701	CG2	ILE D	16	44.319	57.455	34.414	1.00	107.28
	4702 4703	CG1 CD1	ILE D	16	46.303	57.587	32.876	1.00	107.28
20	4704	CD	ILE D	16 16	46.295 45.380	59.099 54.992	32.854 31.754	1.00 1.00	107.28
	4705	0	ILE D	16	46.492	54.553	31.461	1.00	65.25 65.25
	4706.	N	PHE D	17	44.373	55.117	30.905	1.00	82.89
	4707 4708	CA CB	PHE D PHE D	17 17	44.429	54.750	29.509	1.00	82.89
25	4709	CG	PHE D	17	43.011 42.550	54.508 53.099	29.030 29.186	1.00 1.00	73.74 73.74
	4710	CD1	PHE D	17	41.245	52.822	29.578	1.00	73.74 73.74
	4711	CD2	PHE D	17	43.379	52.052	28.825	1.00	73.74
	4712 4713	CE1 CE2	PHE D PHE D	17 17	40.779 42.918	51.529 50.741	29.625 28.866	1.00	73.74
30	4714	cz	PHE D	17	41.609	50.484	29.258	1.00 1.00	73.74 73.74
	4715	C	PHE D	17	45.066	55.8 63	28.677	1.00	82.89
	4716 4717	0 N	PHE D LYS D	17 18	45.154 45.502	57.009	29.117	1.00	82.89
	4718	ČA	LYS D	18	45.502 46.117	55.531 56.516	27.469 26.588	1.00 1.00	90.77 90.77
35	4719	CB	LYS D	18	46.681	55.810	25.357	1.00	139.85
	4720 4721	CG CD	LYS D LYS D	18	47.467	56.691	24.410	1.00	139.85
	4722	CE	LYS D	18 18	48.254 49.094	55.822 56.637	23.441 22.472	1.00 1.00	139.85
	4723	NZ	LYS D	18	48.256	57.533	21.630	1.00	139.85 139.85
40	4724	C	LYS D	18	45.079	57.556	26.156	1.00	90.77
	4725 4726	0 N	LYS D GLY D	18 19	43.975 45.420	57.212	25.731	1.00	90.77
	4727	CA	GLY D	19	44.501	58.832 59.869	26.284 25.859	1.00 1.00	135.30 135.30
45	4728	Ç ,	GLY D	19	43.585	60.458	26.909	1.00	135.30
45	4729 4730	0 N	GLY D	19	42.914	61.451	26.641	1.00	135.30
	4731	ČA	GLU D GLU D	20 20	43.539 42.679	59.863 60.387	28.096 29.158	1.00 1.00	90.73
	4732	СВ	GLU D	20	42.370	59.283	30.165	1.00	90.73 145.66
50	4733	CG	GLU D	20	41.858	58.007	29.497	1.00	145.66
30	4734 4735	CD OE1	GLU D GLU D	20 20	41.421 42.233	56.945	30.491	1.00	145.66
	4736	OE2	GLU D	20	40.265	56.567 56.483	31.363 30.393	1.00 1.00	145.66 145.66
	4737	Č	GLU D	20	43.339	61.593	29.844	1.00	90.73
55	4738 4739	O N	GLU D	20	44.510	61.887	29.590	1.00	90.73
55	4740	CA CA	ASN D ASN D	21 21	42.592 43.163	62.311 63.469	30.682 31.364	1.00	106.51
	4741	CB	ASN D	21	42.409	64.761	31.030	1.00 1.00	106.51 191.80
	4742	CG	ASN D	21	42.014	64.865	29.580	1.00	191.80
60	4743 4744	OD1 ND2	ASN D ASN D	21	42.781	64.543	28.677	1.00	191.80
•	4745	C	ASN D	21 21	40.797 43.127	65.346 63.300	29.365 32.872	1.00 1.00	191.80 106.51
	4746	0	ASN D	21	42.165	62.756	33.424	1.00	106.51
	4747 4740	N CA	VAL D	22	44.170	63. 79 2	33.533	1.00	83.07
65	4748 4749	CA CB	VAL D VAL D	22 22	44.267 45.143	63.727 62.571	34.984	1.00	83.07
	4750	CG1	VAL D	22	45.143 46.555	62.571 62.774	35.425 34.923	1.00 1.00	85.11 85.11
	4751	CG2	VAL D	22	45.134	62.475	36.937	1.00	85.11
	4752 4753	C	VAL D	22	44.885	65.015	35.514	1.00	83.07
70	4754	N	VAL D THR D	22 23	45.701 44.517	65. 6 43 65.401	34.833	1.00	83.07
-		• •		20	 .51/	00.401	36.731	1.00	66.58

	4755 4756 4757	CA CB OG1	THR D THR D THR D	23 23 23	45.024 43.848 43.036	66.635 67.553 67.717	37.318 37.646	1.00	66.58 160.89
5	4758 4759 4760	CG2 C O	THR D THR D THR D	23 23 23	44.344 45.820 45.330	68.902 66.391 65.718	36.477 38.121 38.598	1.00 1.00 1.00	160.89 160.89 66.58
	4761 4762 4763	N CA CB	LEU D LEU D LEU D	24 24 24	47.035 47.810 49.235	66.923 66.708 66.263	39.498 38.705 39.933	1.00 1.00 1.00	66.58 91.98 91.98
10	4764 4765 4766	CG CD1 CD2	LEU D LEU D	24 24 24	49.491 50.891 48.509	65.315 64.750 64.210	39.632 38.471 38.587 38.476	1.00 1.00 1.00	82.54 82.54 82.54
15	4767 4768 4769	C O N	LEU D LEU D THR D	24 24 25	47.882 48.622 47.131	67.967 68.895 67.992	40.785 40.479 41.873	1.00 1.00 1.00 1.00	82.54 91.98 91.98
	4770 4771 4772	CA CB OG1	THR D THR D THR D	25 25 25	47.122 45.754 44.757	69.153 69.300 69.342	42.732 43.385 42.357	1.00 1.00 1.00	89.48 89.48 145.87 145.87
20	4773 4774 4775	CG2 C O	THR D THR D THR D	25 25 25	45.686 48.199 48.404	70.568 69.028 67.956	44.198 43.794 44.359	1.00 1.00 1.00	145.87 145.87 89.48 89.48
25	4776 4777 4778	N CA C	CYS D CYS D CYS D	26 26 26	48.909 49.942 49.298	70.117 70.082 70.358	44.050 45.070 46.407	1.00 1.00 1.00	125.74 125.74 125.74 125.74
23	4779 4780 4781 4782	O CB SG N	CYS D CYS D CYS D	26 26 26	48.415 51.034 52.476	71.196 71.118 70.930	46.512 44.810 45.922	1.00 1.00 1.00	125.74 105.78 105.78
30	4783 4784 4785	CA CB CG	ASN D ASN D ASN D ASN D	27 27 27 27	49.751 49.263 50.450 50.107	69.628 69.743 69.894 69.554	47.416 48.776 49.698	1.00 1.00 1.00	184.56 184.56 249.08
	4786 4787 4788	OD1 ND2 C	ASN D ASN D ASN D	27 27 27 27	49.328 50.683 48.283	68.630 70.281 70.880	51.100 51.334 52.054 49.023	1.00 1.00 1.00 1.00	249.08 249.08 249.08
35	4789 4790 4791	O N CA	ASN D GLY D GLY D	27 28 28	48.686 46.995 45.972	71.988 70.600 71.612	49.365 48.844 49.043	1.00 1.00 1.00	184.56 184.56 249.39 249.39
40	4792 4793 4794	C O N	GLY D GLY D ASN D	28 28 29	44.644 44.494 43.674	71.030 70.609 71.006	48.616 47.470 49.524	1.00 1.00 1.00	249.39 249.39 249.47
	4795 4796 4797 4798	CA CB CG OD1	ASN D ASN D ASN D	29 29 29	42.377 41.619 40.397	70.429 70.112 69.249	49.206 50.497 50.256	1.00 1.00 1.00	249.47 246.79 246.79
45	4799 4800 4801	ND2 C	asn d Asn d Asn d Asn d	29 29 29 29	40.234 39.536 41.494 41.005	68.672 69.146 71.261	49.182 51.262 48.274	1.00 1.00 1.00	246.79 246.79 249.47
50	4802 4803 4804	N CA CB	ASN D ASN D ASN D	30 30 30	41.294 40.437 39.137	70.746 72.538 73.386 73.705	47.265 48.594 47.766	1.00 1.00 1.00	249.47 206.51 206.51
	4805 4806 4807	CG OD1 ND2	ASN D ASN D ASN D	30 30 30	38.302 37.878 38.054	72,469 72,232 71,678	48.518 48.794 49.926 47.757	1.00 1.00 1.00 1.00	210.57 210.57 210.57
55	4808 4809 4810	C O N	ASN D ASN D PHE D	30 30 31	41.073 41.381 41.266	74.685 74.848 75.614	47.297 46.115 48.224	1.00 1.00 1.00	210.57 206.51 206.51 230.41
60	4811 4812 4813 4814	CA CB CG	PHE D	31 31 31	41.829 40.891 39.472	76.899 78.020 77.878	47.860 48.330 47.828	1.00 1.00 1.00	230.41 249.56 249.56
00	4815 4816 4817	CD1 CD2 CE1 CE2	PHE D PHE D	31 31 31	38.588 39.030 37.283	76.991 78.608 76.839	48.440 46.725 47.969	1.00 1.00 1.00	249.56 249.56 249.56
65	4818 4819 4820	CZ C	PHE D PHE D PHE D PHE D	31 31 31 31	37.727 36.853 43.249	78.463 77.574 77.132	46.245 46.866 48.360	1.00 1.00 1.00	249.56 249.56 230.41
	4821 4822 4823	N CA CB	PHE D PHE D PHE D	32 32 32	43.542 44.122 45.531 48.392	76.994 77.486 77.753 76.753	49.552 47.416 47.683	1.00 1.00 1.00	230.41 186.13 186.13
70	4824	CG	PHE D	32	47.810	76.726	46.925 47.381	1.00 1.00	237.35 237.35

	4005	004	0115 5						
	4825 4826	CD1 CD2	PHE D PHE D	32 32	· 48.121 48.835	76.283 77.167	48.659	1.00	237.35
	4827	CE1	PHE D	32	49.434	76.277	46.552 49.112	1.00 1.00	237.35
_	4828	CE2	PHE D	32	50.156	77.166	46.998	1.00	237.35 237.35
5	4829	cz	PHE D	32	50.454	76.719	48.286	1.00	237.35
	4830	C	PHE D	32	45.909	79.173	47.251	1.00	186.13
	4831 4832	O N	PHE D GLU D	32 33	45.122	79.856	46.601	1.00	186.13
	4833	CA	GLU D	33	47.117 47.539	79.617 80.969	47.595 47.225	1.00 1.00	249.49
10	4834	СВ	GLU D	33	47.683	81.860	48.457	1.00	249.49 249.38
	4835	CG	GLU D	33	47.919	83.321	48.090	1.00	249.38
	4836	CD	GLU D	33	46.730	83.912	47.362	1.00	249.38
	4837 4838	OE1 OE2	GLU D	33	45.593	83.561	47.740	1.00	249.38
15	4839	C	GLU D	33 33	46.914 48.822	84.731 81.120	46.433	1.00	249.38
	4840	ŏ	GLU D	33	48.826	81.765	46.422 45.372	1.00 1.00	249.49
	4841	Ň	VAL D	34	49.918	80.566	46.929	1.00	249.49 207.78
	4842	CA	VAL D	34	51.194	80.698	46.247	1.00	207.78
20	4843	CB	VAL D	34	52.284	79.859	46.944	1.00	207.37
20	4844 4845	CG1	VAL D	34	53.608	80.005	46.212	1.00	207.37
	4846	CG2 C	VAL D VAL D	34 34	52.437 51.130	80.316	48.384	1.00	207.37
	4847	ŏ	VAL D	34	50.333	80. 333 79.492	44.770 44.343	1.00 1.00	207.78
	4848	Ň	SER D	35	51.966	81.007	43.992	1.00	207.78 228.15
25	4849	CA	SER D	35	52.043	80.778	42.563	1.00	228.15
	4850	CB	SER D	35	51.944	82.104	41.810	1.00	249.21
	4851	og	SER D	35	53.093	82.901	42.038	1.00	249.21
	4852 4853	C	SER D SER D	35 35	53.386 53.703	80.116	42.275	1.00	228.15
30	4854	Ň	SER D	36	54.1 7 7	79.813 79.906	41.126 43.326	1.00 1.00	228.15 238.59
	4855	CA	SER D	36	55.481	79.265	43.185	1.00	238.59
	4856	СВ	SER D	36	56.552	80.002	43.997	1.00	200.88
	4857	og	SER D	36	56.368	79.808	45.389	1.00	200.88
35	4858 4859	C	SER D SER D	36	55.395	77.821	43.653	1.00	238.59
55	4860	Ň	SER D THR D	36 37	55.568 55.115	77.519 76.935	44.835 42.706	1.00	238.59
	4861	ĊA	THR D	37	55.004	75.514	42.974	1.00 1.00	119.38 119.38
	4862	СВ	THR D	37	53.561	75.034	42.738	1.00	138.47
40	4863	OG1	THR D	37	52.664	75.794	43.557	1.00	138.47
40	4864 4865	CG2 C	THR D	37	53.426	73.568	43.078	1.00	138.47
	4866	ŏ	THR D THR D	37 37	55.950 56.054	74.838 75.258	41.992	1.00	119.38
	4867	Ň	LYS D	38	56.653	73.808	40.841 42.446	1.00 1.00	119.38 140.44
	4868	CA	LYS D	38	57.594	73.098	41.585	1.00	140.44
45	4869	СВ	LYS D	38	58.938	72.982	42.288	1.00	200.36
	4870 4871	CG	LYS D	38	59.508	74.309	42.714	1.00	200.36
	4872	CD CE	LYS D Lys d	38 38	60.837 61.449	74.125	43.415	1.00	200.36
	4873	NZ	LYS D	38	62.770	75.465 75.308	43.766 44.427	1.00 1.00	200.36
50	4874	C	LYS D	38	57.100	71.701	41.218	1.00	200.36 140.44
	4875	0	LYS D	38	56.507	71.013	42.045	1.00	140.44
	4876	N	TRP D	39	57.341	71.284	39.976	1.00	125.62
	4877 4878	CA CB	TRP D	39	56.934	69.953	39.520	1.00	125.62
55	4879	CG	TRP D	39 39	55.830 54.540	70.028 70.582	38.470	1.00	111.13
	4880	CD2	TRP D	39	53.645	69.978	38.973 39.915	1.00 1.00	111.13
	4881	CE2	TRP D	39	52.567	70.867	40.090	1.00	111.13
	4882	CE3	TRP D	39	53.651	68.776	40.628	1.00	111.13
60	4883	CD1	TRP D	39	53.984	71.774	38.628	1.00	111.13
UU	4884 4885	NE1 CZ2	TRP D	39 39	52.798	71.953	39.295	1.00	111.13
	4886	CZ3	TRP D	39	51.503 52.589	70.588 68.503	40.948 41.482	1.00	111.13
	4887	CH2	TRP D	39	51.531	69.405	41.633	1.00 1.00	111.13 111.13
C =	4888	С	TRP D	39	58.115	69.240	38.913	1.00	125.62
65	4889	0	TRP D	39	58.809	69. 7 97	38.077	1.00	125.62
	4890 4891	N CA	PHE D	40	58.331	68.000	39.318	1.00	94.48
	4892	CB	PHE D PHE D	40 40	59.458 60.476	67.260 66.076	38.800	1.00	94.48
	4893	ČĠ	PHE D	40	60.475 60.977	66.976 68.203	39.910 40.607	1.00	162.61
70	4894	CD1	PHE D	40	60.217	68.816	41.594	1.00 1.00	162.61 162.61
									102.01

PCT/US99/26203

	4895	CD2	PHE D	40	62,222	68.734	40.292	1.00	162.61
	4896	CE1	PHE D	40	60.687	69.941	42.264	1.00	162.61
	4897	CE2	PHE D	40	62.705	69.859	40.953	1.00	162.61
_	4898	CZ	PHE D	40	61.934	70.465	41.945	1.00	162.61
5	4899	C	PHE D	40	59.063	65.951	38.152	1.00	94.48
	4900	0	PHE D	40	59.061	64.906	38.803	1.00	94.48
	4901 4902	N CA	HIS D HIS D	41	58.727	66.006	36.869	1.00	72.94
	4903	CB	HIS D	41 41	58.368 57.649	64.797	36.133	1.00	72.94
10	4904	CG	HIS D	41	57.262	65.192 64.034	34.848 33.991	1.00	108.26
	4905	CD2	HIS D	41	57.305	63.866	32.649	1.00 1.00	108.26
	4906	ND1	HIS D	41	56.717	62.879	34.507	1.00	108.26 108.26
	4907	CE1	HIS D	41	56.441	62.049	33.519	1.00	108.26
	4908	NE2	HIS D	41	56.788	62.625	32.381	1.00	108.26
15	4909	С	HIS D	41	59.642	63.973	35.816	1.00	72.94
	4910	0	HIS D	41	60.482	64.384	35.014	1.00	72.94
	4911	N	ASN D	42	59.770	62.805	36.445	1.00	79.39
	4912	CA CB	ASN D	42	60.939	61.934	36.277	1.00	79.39
20	4913 4914	CG	ASN D ASN D	42	61.153	61.JeJ	34.808	1.00	100.05
20	4915	OD1	ASN D	42 42	60.141 58.962	60.504 60.635	34.327	4.00	100.05
	4916	ND2	ASN D	42	60.578	59.502	34.637 33.560	1.00	100.05
	4917	C	ASN D	42	62.190	62.653	36.783	1.00 1.00	100.05 79.39
	4918	ō	ASN D	42	63.298	62.386	36,318	1.00	79.39 79.39
25	4919	N	GLY D	43	62.013	63.562	37.739	1.00	194.33
	4920	CA	GLY D	43	63.147	64.294	38.279	1.00	194.33
	4921	С	GLY D	43	63.397	65.624	37.584	1.00	194.33
	4922	0	GLY D	43	63.744	66.616	38.226	1.00	194.33
30	4923	N	SER D	44	63.221	65.644	36.267	1.00	226.19
30	4924	CA CB	SER D	44	63.422	66.852	35.476	1.00	226.19
	4925 4926	OG	SER D SER D	44 44	63.315	66.520	33.987	1.00	149.84
	4927	C	SER D	44	64.180 62.376	65.450 67.899	33.639	1.00	149.84
	4928	ŏ	SER D	44	61.179	67.617	35.837 35.812	1.00 1.00	226.19
35	4929	N	LEU D	45	62.824	69.107	36.172	1.00	226.19 151.08
	4930	CA	LEU D	45	61.897	70.180	36.531	1.00	151.08
	4931	СВ	LEU D	45	62.673	71.473	36.830	1.00	168.08
	4932	CG	LEU D	45	61.854	72.699	37.259	1.00	168.08
40	4933	CD1	LEU D	45	60.980	72.345	38.451	1.00	168.08
40	4934	CD2	LEU D	45	62.788	73.853	37.607	1.00	168.08
	4935 4936	C	LEU D	45 45	60.885	70.422	35.398	1.00	151.08
	4937	N	SER D	45 46	61.215 59.650	70.281	34.219	1.00	151.08
	4938	ČA	SER D	46	58.614	70.772 71.032	35.755 34.762	1.00	118.65
45	4939	CB	SER D	46	57.279	70.467	35.236	1.00 1.00	118.65 145.92
	4940	OG	SER D	46	56.288	70.641	34.240	1.00	145.92
	4941	C	SER D	46	58.499	72.537	34.569	1.00	118.65
	4942	0	SER D	46	59.012	73.306	35.378	1.00	118.65
50	4943	N	GLU D	47	57.828	72.965	33.505	1.00	181.92
50	4944	CA	GLU D	47	57.679	74.395	33.255	1.00	181.92
	4945	CB	GLU D	47	57.725	74.692	31.746	1.00	232.55
	4946 4947	CD	GLU D	47 47	58.747	73.882	30.951	1.00	232.55
	4948	OE1	GLU D	47 47	58.494 57.657	73.918 73.130	29.437	1.00	232.55
55	4949	OE2	GLU D	47	59.123	73.130 74.749	28.947 28.747	1.00	232.55
	4950	Č	GLU D	47	56.398	74.999	33.858	1.00 1.00	232.55 181.92
	4951	O	GLU D	47	56.185	76.203	33.732	1.00	181.92
	4952	N	GLU D	48	55.538	74.196	34.492	1.00	100.90
60	4953	CA	GLU D	48	54.330	74.777	35.104	1.00	100.90
60	4954	CB	GLU D	48	53.184	73.753	35.227	1.00	175.62
	4955	CG	GLU D	48	51.945	74.246	36.025	1.00	175.62
	4956 4957	CD OE1	GLU D	48	51.173	75.384 76.147	35.355	1.00	175.62
	4957 4958	OE2	GLU D	48 48	50.544 51.103	75.147 76.517	34.300	1.00	175.62
65	4959	C	GLU D	48 48	51.193 54.698	76.517 75.309	35.887 36.490	1.00	175.62
	4960	ŏ	GLU D	48	55.879	74.868	37.096	1.00 1.00	100.90 100.90
	4961	Ň	THR D	49	53.927	76.275	36.977	1.00	145.22
	4962	CA	THR D	49	54.186	76.860	38.287	1.00	145.22
70	4963	CB	THR D	49	54.710	78.308	38.155	1.00	156.90
70	4964	OG1	THR D	49	53.774	79.094	37.405	1.00	156.90

	4965	CG2	THR D	49	- 56.059	78.319	37.442	1.00	150.00
	4966	C	THR D	49	52.921	76.841	39.150	1.00	156.90 145.22
	4967	Ŏ	THR D	49	53.002	76.780	40.384	1.00	145.22
_	4968	Ν.	ASN D	50	51.757	76.881	38.500	1.00	138.33
5	4969	ÇA	ASN D	50	50.486	76.844	39.213	1.00	138.33
	4970	СВ	ASN D	50	49.323	76.826	38.220	1.00	234.43
	4971	CG OD1	ASN D ASN D	50	47.991 47.868	77.129 77.026	38.880	1.00	234.43
	4972 4973	ND2	ASN D	50 50	47.800 46.989	77.490	40.100 38.081	1.00 1.00	234.43 234.43
10	4974	C	ASN D	50	50.480	75.564	40.054	1.00	138.33
	4975	Ö	ASN D	50	51.104	74.574	39.683	1.00	138.33
	4976	N	SER D	51	49.782	75.578	41.183	1.00	192.24
	4977	CA	SER D	51	49.733	74.400	42.046	1.00	192.24
15	4978	CB	SER D	51	49.042	74.734	43.376	1.00	111.18
13	4979 4980	og C	SER D SER D	51 51	47.655 49.023	74.994 73.213	43.211 41.399	1.00 1.00	111.18
	4981	ŏ	SER D	51	49.166	73.213 72.078	41.848	1.00	192.24 192.24
	4982	Ň	SER D	52	48.252	73.470	40.351	1.00	99.05
	4983	CA	SER D	52	47.526	72.400	39.677	1.00	99.05
20	4984	CB	SER D	52	46.041	72.765	39.522	1.00	120.15
	4985	OG	SER D	52	45.402	72.880	40.781	1.00	120.15
	4986	C	SER D	52	48.147	72.145	38.314	1.00	99.05
	4987 4988	0 N	SER D LEU D	52 53	48.052 48.797	72.970 70.997	37.410 38.183	1.00	99.05
25	4989	CA	LEU D	53	49.443	70.602	36.938	1.00 1.00	107.39 107.39
	4990	CB	LEU D	53	50.774	69.910	37.246	1.00	80.33
	4991	CG	LEU D	53	51.398	68.972	36.203	1.00	80.33
	4992	CD1	LEU D	53	51.298	69.580	34.817	1.00	80.33
20	4993	CD2	LEU D	53	52.856	68.675	36.589	1.00	80.33
30	4994 4005	C	LEU D	53	48.548	69.654	36.158	1.00	107.39
	4995 4996	0 N	ASN D	53 54	48.472 47.876	68.474 70.159	36.476 35.130	1.00 1.00	107.39 103.21
	4997	CA	ASN D	54	46.989	69.314	34. 33 9	1.00	103.21
	4998	CB	ASN D	54	45.977	70.162	33.573	1.00	126.61
35	4999	CG	ASN D	54	44.932	70.755	34.475	1.00	126.61
	5000	OD1	ASN D	54	44.260	70.038	35.217	1.00	126.61
	5001	ND2	ASN D	54	44.781	72.072	34.420	1.00	126.61
	5002 5003	C O	ASN D ASN D	54 54	47.732 48.882	68.434 68.690	33.362 33.026	1.00	103.21
40	5003	Ň	ILE D	55	40.002 47.056	67.381	32.921	1.00 1.00	103.21 179.18
	5005	ĊA	ILE D	55	47.601	66.449	31.947	1.00	179.18
	5006	CB	ILE D	55	48.061	65,127	32.606	1.00	94.31
	5007	CG2	ILE D	5 5	48.187	64.027	31.558	1.00	94.31
45	5008	CG1	ILE D	55	49.393	65.356	33.324	1.00	94.31
43	5009 5010	CD1 C	ILE D	55	49.946	64.146	34.029	1.00	94 31
	5011	ŏ	ILE D	55 55	46.473 45.402	66.173 65.719	30.975 31.373	1.00 1.00	175.18 179.18
	5012	Ň	VAL D	56	46.701	66.476	29.704	1.00	148.36
	5013	CA	VAL D	56	45.674	66.254	28.704	1.00	148.36
50	5014	CB	VAL D	56	45.589	67.433	27.737	1.00	191.19
	5015	CG1	VAL D	56	44.260	67.393	26.992	1.00	191.19
	5016	CG2	VAL D	56 50	45.729	68.734	28.509	1.00	191.19
	5017 5018	C O	VAL D VAL D	56 56	45.998 46.797	64.975 64.180	27.956 28.445	1.00 1.00	148.36 148.36
55	3019	Ň	ASN D	57	45.386	64.774	26.789	1.00	142.96
	5020	CA	ASN D	57	15.604	63.560	25.999	1.00	142.96
	5021	CB	ASN D	57	45.673	63.895	24.509	1.00	249.24
	5022	CG	ASN D	57	44.331	64.323	23.952	1.00	249.24
60	5023	OD1	ASN D	57	43.331	63.617	24.101	1.00	249.24
00	5024 5025	ND2	asn d Asn d	57 57	44.298	65.482 63.845	23.307	1.00	249.24
	5025 5026	C O	ASN D	57 57	46.861 47.956	62.815 63.052	26.436 25.919	1.00 1.00	142.96 142.96
	5027	Ň	ALA D	58	46.683	61.917	27.403	1.00	155.81
.	5028	CA	ALA D	58	47.775	61.140	27.966	1.00	155.81
65	5029	CB	ALA D	58	47.245	60.191	29.002	1.00	45.44
	5030	C	ALA D	58	48.595	60.375	26.939	1.00	155.81
	5031	0	ALA D	58	48.086	59.524	26.214	1.00	155.81
	5032 5033	N CA	LYS D LYS D	59 59	49.881 50.807	60.690 60.036	26.890 25.070	1.00	75.94
70	5034	CB	LYS D	59 59	50.607 51.654	61.085	25.979 25.248	1.00 1.00	75.94 205.66
		- -							-~.~

	5035	CG	LYS D	59	50.830	62.088	24.439	1.00	205.66
	5036	CD	LYS D	59	51.689	63.187	23.829	1.00	205.66
	5037	CE	LYS D	59	50.838	64.174	23.036	1.00	
	5038	NZ	LYS D	59	51.652	65.278	22.452		205.66
5	5039	Ċ	LYS D	59	51.673	59.164	26.886	1.00	205.66
•	5040	ŏ	LYS D	59				1.00	75.94
	5041	Ň			51.945	59.548	28.028	1.00	75.94
			PHE D	60	52.082	57.991	26.398	1.00	73.11
	5042	CA	PHE D	60	52.916	57.070	27.183	1.00	73.11
• •	5043	CB	PHE D	60	53.521	56.025	26.277	1.00	111.86
10	5044	CG	PHE D	60	52.512	55.131	25.662	1.00	111.86
	5045	CD1	PHE D	60	52.745	54.540	24.431	1.00	
	5046	CD2	PHE D	60	51.323	54.863	26.314	1.00	111.86
	5047	CE1	PHE D	60	51.810				111.86
	5048	CE2				53.690	23.853	1.00	111.86
15			PHE D	60	50.379	54.018	25.750	1.00	111.86
13	5049	CZ	PHE D	60	50.622	53.429	24.517	1.00	111.86
	5050	С	PHE D	60	54.026	57.782	27.946	1.00	73.11
	5051	0	PHE D	60	54.401	57.368	29.037	1.00	73.11
	5052	N	GLU D	61	54.544	58.863	27.369	1.00	133.04
	5053	CA	GLU D	61	55.611	59.639	27.993	1.00	133.04
20	5054	CB	GLU D	61	56.112	60.736	27.046	1.00	
	5055	CG	GLU D	61					249.40
	5056	CD	GLU D		56.707	60.232	25.750	1.00	249.40
				61	55.711	59.447	24.926	1.00	249.40
	5057	OE1	GLU D	61	54.616	59.981	24.643	1.00	249.40
0.5	5058	OE2	GLU D	61	56.023	58.296	24.561	1.00	249.40
25	5059	С	GLU D	61	55.162	60.298	29.289	1.00	133.04
	5060	0	GLU D	61	55.995	60.638	30.124	1.00	133.04
	5061	N	ASP D	62	53.854	60.493	29.452	1.00	
	5062	CA	ASP D	62	53.344	61.130			85.82
	5063	CB	ASP D	62			30.659	1.00	85.82
30	5064	CG			51.887	61.546	30.471	1.00	150.56
50			ASP D	62	51.694	62.436	29.258	1.00	150.56
	5065	OD1	ASP D	62	52.584	63.274	28.983	1.00	150.56
	5066	OD2	ASP D	62	50.650	62.302	28.585	1.00	150.56
	5067	С	ASP D	62	53.484	60.179	31.838	1.00	85.82
	5068	0	ASP D	62	53.464	60.605	32.999	1.00	85.82
35	5069	N	SER D	63	53.636	58.888	31.532	1.00	75.53
	5070	CA	SER D	63	53.798	57.858	32.566		
	5071	CB	SER D	63				1.00	75.53
	5072	OG			53.958	56.471	31.933	1.00	120.69
			SER D	63	52.776	56.060	31.271	1.00	120.69
40	5073	Ç	SER D	63	55.064	58.219	33.303	1.00	75.53
40	5074	0	SER D	63	56.071	58.44 0	32.671	1.00	75.53
	5075	N	GLY D	64	55.038	58.291	34.624	1.00	67.79
	5076	CA	GLY D	64	56.262	58.644	35.318	1.00	67.79
	5077	С	GLY D	64	56.113	58.959	36.798	1.00	67.79
	5078	Ō	GLY D	64	55.060	58.708	37.391	1.00	
45	5079	Ň	GLU D	65	57.173	59.500			67.79
	5080	CA	GLU D				37.396	1.00	63.91
				65	57.212	59.843	38.817	1.00	63.91
	5081	CB	GLU D	65	58.542	59.353	39.392	1.00	198.27
	5082	CG	GLU D	65	58.869	59.830	40.778	1.00	198.27
~^	5083	CD	GLU D	65	60.319	59.576	41.129	1.00	198.27
50	5084	OE1	GLU D	65	61.203	60.162	40.465	1.00	198.27
	5085	OE2	GLU D	65	60.576	58.786	42.061	1.00	198.27
	5086	С	GLU D	65	57.098	61.355	38.943	1.00	
	5087	Ö	GLU D	65					63.91
	5088	Ň	TYR D		57.862	62.078	38.322	1.00	63.91
55	5089			66	56.151	61.849	39.727	1.00	104.89
<i>J</i> J		CA	TYR D	66	55.995	63.295	39.869	1.00	104.89
	5090	СВ	TYR D	66	54.621	63.739	39.384	1.00	61.05
	5091	CG	TYR D	66	54.348	63.543	37.922	1.00	61.05
	5092	CD1	TYR D	66	54.057	62.291	37.403	1.00	61.05
	5093	CE1	TYR D	66	53.721	62.142	36.065	1.00	61.05
60	5094	CD2	TYR D	66	54.307	64.633	37.065	1.00	
	5095	CE2	TYR D						61.05
	5096			66 66	53.972	64.489	35.737	1.00	61.05
		CZ	TYR D	66	53.679	63.253	35.239	1.00	61.05
	5097	ОН	TYR D	66	53.338	63.149	33.911	1.00	61.05
CF	5098	Ç	TYR D	66	56,119	63.743	41.314	1.00	104.89
65	5099	0	TYR D	66	55.990	62.923	42.228	1.00	104.89
	5100	N	LYS D	67	56.343	65.046	41.518	1.00	107.31
	5101	CA	LYS D	67	56.437	65.618	42.867	1.00	
	5102	CB	LYS D	67	57.700				107.31
	5103	cg	LYS D	67		65.134 65.307	43.562	1.00	121.51
70	5104	CD			58.926	65.307	42.721	1.00	121.51
, 0	5104	CU	LYS D	67	60.124	64.712	43.416	1.00	121.51

	5105 5106	CE NZ	LYS D	67	61.319 62.482	64.708 64.056	42.491 43.140	1.00 1.00	121.51 121.51
	5107 5108	C	LYS D		56.419 56.758	67.137	42.839	1.00	107.31
5	5109	Ň	CYS		55.994	67.744 67.747	41.836 43.937	1.00 1.00	107.31
	5110	CA	CYS D	68	55.962	69.190	44.011	1.00	110.81 110.81
	5111	C	CYS D		56.694	69.634	45.260	1.00	110.81
	5112 5113	O CB	CYS D		56.922 54.518	68.842 69.727	46.170	1.00	110.81
10	5114	SG	CYS		53.384	69.216	43.988 45.310	1.00 1.00	140.31 140.31
	5115	N	GLN D	69	57.093	70.900	45.274	1.00	126.93
	5116	CA	GLN D		57.804	71.490	46.396	1.00	126.93
	5117 5118	CB CG	GLN D		59.300 60.185	71.191 72.102	46.281 47.115	1.00	112.91
15	5119	CD	GLN D		61.665	71.867	46.875	1.00 1.00	112.91 112.91
	5120	OE1	GLN D	69	62.131	71.871	45.730	1.00	112.91
	5121 5122	NE2	GLN D		62.416	71.667	47.959	1.00	112.91
	5122	C O	GLN D		57.566 57.314	72.990 73.542	46.341 45.269	1.00	126.93
20	5124	Ň	HIS D		57.642	73.652	47.488	1.00 1.00	126.93 191.71
	5125	CA	HIS D		57.429	75.090	47.528	1.00	191.71
	5126 · 5127	CB CG	HIS D		56.372	75.434	48.577	1.00	178.35
	5128	CD2	HIS D		54.997 54.315	74.961 73.848	48.219 48.585	1.00	178.35
25	5129	ND1	HIS D		54.173	75.648	47.353	1.00 1.00	178.35 178.35
	5130	CE1	HIS D		53.041	74.981	47.202	1.00	178.35
	5131 5132	NE2 C	HIS D		53.101	73.886	47.940	1.00	1 78.3 5
	5133	ŏ	HIS D		58.711 59.813	75.856 75.299	47.808 47.784	1.00	191.71
30	5134	N	GLN D	71	58.553	77.145	48.068	1.00 1.00	191.71 249.37
	5135	CA	GLN D		59.681	78.018	48.338	1.00	249.37
	5136 5137	CB CG	GLN D		59.161	79.419	48.681	1.00	212.46
	5138	CD	GLN D		60.101 60.527	80.540 80.432	48.260 46.806	1.00 1.00	212.46
35	5139	OE1	GLN D	71	59.736	80.661	45.894	1.00	212.46 212.46
	5140	NE2	GLN D		61.786	80.066	46.587	1.00	212.46
	5141 5142	C	GLN D		60.570 61.775	77.474	49.462	1.00	249.37
	5143	Ň	GLN D		59.974	77.297 77.195	49.269 50.622	1.00 1.00	249.37 156.64
40	5144	CA	GLN D	72	60.728	76.683	51.771	1.00	156.64
	5145 5146	CB	GLN D		60.738	77.728	52.895	1.00	249.31
	5146 5147	CD	GLN D		61.596 61.612	77.360 78.445	54.104 55.460	1.00	249.31
	5148	OE1	GLN D		62.001	79.584	55.168 54.904	1.00 1.00	249.31 249.31
45	5149	NE2	GLN D	72	61.187	78.096	56.378	1.00	249.31
	5150	C	GLN D		60.149	75.374	52.302	1.00	156.64
	5151 5152	O N	GLN D VAL D	72 73	59.772 60.084	75.277 74.362	53.472	1.00	156.64
	5153	CA	VAL D		59.530	74.362 73.078	51.446 51.852	1.00 1.00	234.28 234.28
50	5154	CB	VAL D		58.026	73.002	51.529	1.00	131.77
	5155 5156	CG1	VAL D		57.398	71.832	52.244	1.00	131.77
	5157	CG2 C	VAL D		57.350 60.224	74.292 71.930	51.910	1.00	131.77
	5158	ŏ	VAL D		60.652	72.060	51.141 49.995	1.00 1.00	234.28 234.28
55	5159	N _.	ASN D	74	60.337	70.802	51.824	1.00	160.29
	5160 5161	CA CB	ASN D		60.971	69.646	51.228	1.00	160.29
	5162	CG	ASN D		61.437 62.337	68.687 69.366	52.321	1.00	140.71
	5163	OD1	ASN D		63.216	70.152	53.332 52.957	1.00 1.00	140.71 140.71
60	5164	ND2	ASN D	74	62.130	69.065	54.613	1.00	140.71
	5165 5166	C	ASN D		59.985	68.964	50.286	1.00	160.29
	5167	Ň	ASN D GLU D	74 75	58.839 60.446	68.692 68.711	50.653	1.00	160.29
	5168	CA	GLU D		59.644	68.074	49.064 48.028	1.00 1.00	155.73 155.73
65	5169	CB	GLU D	75	60.555	67.631	46.881	1.00	134.99
	5170 5171	CD	GLU D	75 75	61.940	67.190	47.322	1.00	134.99
	5172	OE1	GLU D	75 75	62.884 63.056	66.978 67.916	46.149 45.240	1.00	134.99
70	5173	OE2	GLU D	75 75	63.460	65.875	45.340 46.038	1.00 1.00	134.99 134.99
70	5174	С	GLU D	75	58.794	66.907	48.520	1.00	155.73
						•			

	5175 5176	O N	GLU D SER D	75 - 76	59.207 57.601	66.137 66.792	49.385 47.946	1.00	155.73
	5177	ČA	SER D	76	56.635	65.760	48.302	1.00 1.00	91.19
	5178	CB	SER D	76	55.314	66.052	47.619	1.00	91.19 86.66
5	5179	OG	SER D	76	55.477	65.917	46.224	1.00	86.66
	5180	C	SER D	76	57.050	64.349	47.909	1.00	91.19
	5181	0	SER D	76	57.892	64.165	47.020	1.00	91.19
	5182	N CA	GLU D	77	56.431	63.362	48.562	1.00	100.72
10	5183 5184	CA CB	GLU D GLU D	77 77	56.701 55.971	61.959	48.272	1.00	100.72
10	5185	CG	GLU D	77	56.457	61.046 61.191	49.259 50.694	1.00 1.00	188.13
	5186	CD	GLU D	 77	57.912	60.781	50.876	1.00	188.13 188.13
	5187	OE1	GLU D	77	58.637	60.666	49.867	1.00	188.13
	5188	OE2	GLU D	77	58.343	60.589	52.036	1.00	188.13
15	5189	Ç	GLU D	77	56.203	61.715	46.857	1.00	100.72
	5190	0	GLU D	77	55.012	61.851	46.588	1.00	100.72
	5191 5192	N CD	PRO D PRO D	78 78	57.108 59.577	61.380	45.928	1.00	89.58
	5193	CA	PRO D	78	58.577 56.752	61.416 61.125	46.096 44.532	1.00 1.00	142.24
20	5194	CB	PRO D	78	58.018	60.508	43.955	1.00	89.58 142.24
	5195	CG	PRO D	78	59.097	61.270	44.669	1.00	142.24
	5196	С	PRO D	78	55.529	60.249	44.351	1.00	89.58
	5197	Q.	PRO D	78	55.169	59.471	45.234	1.00	89.58
25	5198	N	VAL D	79	54.889	60.397	43.201	1.00	92.62
23	5199 5200	CA CB	VAL D VAL D	79 79	53.713 52.466	59.620	42.893	1.00	92.62
	5200 5201	CG1	VAL D	79 79	51.284	60.484 59.785	42.999 42.333	1.00 1.00	66.56
	5202	CG2	VAL D	79	52.177	60.763	44.458	1.00	66.56 66.56
	5203	C	VAL D	79	53.834	59.092	41.483	1.00	92.62
30	5204	0	VAL D	79	54.122	59.880	40.566	1.00	92.62
	5205	N	TYR D	80	53.625	57.782	41.295	1.00	61.19
	5206	CA	TYR D	80	53.757	57.256	39.952	1.00	61.19
	5207 5208	CB CG	TYR D TYR D	80 80	54.372 54.869	55.878 55.534	39.936	1.00	249.26
35	5209	CD1	TYR D	80	55.895	56.275	38.557 37.979	1.00 1.00	249.26 249.26
	5210	CE1	TYR D	80	56.370	55.971	36.708	1.00	249.26
	5211	CD2	TYR D	80	54.335	54.491	37.816	1.00	249.26
	5212	CE2	TYR D	80	54.829	54.208	36.532	1.00	249.26
40	5213	CZ	TYR D	80	55.822	54.920	35.993	1.00	249.26
40	5214 5215	OH C	TYR D TYR D	80	56.359	54.647	34.755	1.00	249.26
	5216	ŏ	TYR D	80 80	52.471 51.448	57.184 56.804	39.194 39.737	1.00 1.00	61.19
	5217	Ň	LEU D	81	52.529	57.540	37.924	1.00	61.19 59.82
	5218	CA	LEU D	81	51.354	57.492	37.090	1.00	59.82
45	5219	СВ	LEU D	81	51.089	58.875	36.535	1.00	66.30
	5220	CG	LEU D	81	49.972	58.868	35.515	1.00	68.30
	5221	CD1	LEU D	81	48.705	58.435	36.202	1.00	66.30
	5222 5223	CD2 C	LEU D	81 81	49.808 51.664	60.240	34.932	1.00	66.30
50	5224	ŏ	LEU D	81	52.715	56.531 56.663	35.945 35.333	1.00 1.00	59.82 59.82
	5225	Ň	GLU D	82	50.795	55.561	35.658	1.00	81.20
	5226	CA	GLU D	82	51.069	54.640	34.557	1.00	81.20
	5227	CB	GLU D	82	51.229	53.211	35.072	1.00	125.93
E E	5228	CG	GLU D	82	52.081	52.353	34.149	1.00	125.93
55	5229	CD	GLU D	82	52.264	50.938	34.661	1.00	125.93
	5230 5231	OE1 OE2	GLU D	82 82	52.389 52.299	50.771	35.897	1.00	125.93
	5232	C	GLU D	82	49.959	50.001 54.695	33.829 33.498	1.00 1.00	125.93
	5233	ŏ	GLU D	82	48.765	54.633	33.821	1.00	81.20 81.20
60	5234	N	VAL D	83	50.348	54.809	32.230	1.00	74.09
	5235	CA	VAL D	83	49.379	54.891	31.140	1.00	74.09
	5236	CB	VAL D	83	49.747	56.013	30.177	1.00	86.03
	5237 5238	CG1	VAL D	83	48.810	55.997	28.998	1.00	86.03
65	5238 5239	CG2 C	VAL D VAL D	83 83	49.675 49.250	57.340 53.603	30.895	1.00	86.03
	5240	ŏ	VAL D	83	50.237	53.603 53.000	30.340 29.949	1.00 1.00	74.09 74.09
	5241	Ň	PHE D	84	48.023	53.191	30.067	1.00	81.44
	5242	CA	PHE D	84	47.811	51.957	29.331	1.00	81.44
70	5243	CB	PHE D	84	47.087	50.944	30.191	1.00	68.59
70	5244	CG	PHE D	84	47.803	50.598	31.437	1.00	68.59

 \cdot ; \cdot

	5245	CD1	PHE D	84	47.835	51.485	32,486	1.00	60 50
	5246	CD2	PHE D	84	48.418	49.359	31.583	1.00	68.59
	5247	CE1	PHE D	84	48.470	51.153	33.667	1.00	68.59 68.59
_	5248	CE2	PHE D	84	49.058	49.016	32.765	1.00	68.59
5	5249	CZ	PHE D	84	49.078	49.917	33.809	1.00	68.59
	5250	С	PHE D	84	47.029	52.029	28.041	1.00	81,44
	5251	0	PHE D	84	46.324	52.998	27.746	1.00	81.44
	5252	N	SER D	85	47.149	50.938	27.301	1.00	99.54
10	5253	CA	SER D	85	46.462	50.731	26.049	1.00	99.54
10	5254	СВ	SER D	85	47.414	50.901	24.866	1.00	104.48
	5255	QG	SER D	85	46.741	50.652	23.644	1.00	104,48
	5256	Ç	SER D	85	46.015	49.277	26.155	1.00	99.54
	5257	0	SER D	85	46.843	48.362	26.130	1.00	99.54
15	5258	N	ASP D	86	44.713	49.067	26.315	1.00	64.12
13	5259 5260	CA	ASP D	86	44.166	47.724	26.426	1.00	64.12
	5260 5261	CB CG	ASP D	86	44.715	47.030	27.676	1.00	91.49
	5262	OD1	ASP D	86	44.939	45.556	27.454	1.00	91.49
	5263	OD2	ASP D	86 86	43.981	44.874	27.027	1.00	91.49
20	5264	C	ASP D	86	46.065 42.631	17.077	27.697	1.00	91.49
	5265	ŏ	ASP D	86	42.085	47.816 48.907	26.481	1.00	64.12
	5266	Ň	TRP D	87	41.937	46.686	26.673 26.293	1.00	64.12
	5267	ĊA	TRP D	87	40.470	46.689	26.321	1.00	76.92
	5268	CB "	TRP D	87	39.893	45.330	25.950	1.00 1.00	76.92
25	5269	CG	TRP D	87	39.745	45.196	24.519	1.00	235.26
	5270	CD2	TRP D	87	40.716	44.672	23.629	1.00	235.26 235.26
	5271	CE2	TRP D	87	40.219	44.865	22.334	1.00	235.26
	5272	CE3	TRP D	87	41.945	44.025	23.805	1.00	235.26
	5273	CD1	TRP D	87	38.730	45.693	23.748	1.00	235.26
30	5274	NE1	TRP D	87	39.014	45.491	22.409	1.00	235.26
	5275	CZ2	TRP D	87	40.942	44.480	21.244	1.00	235.26
	5276	CZ3	TRP D	87	42.651	43.619	22.683	1.00	235.26
	5277	CH2	TRP D	87	42.147	43.865	21.422	1.00	235.26
25	5278	Ç	TRP D	87	39.956	47.074	27.680	1.00	76.92
35	5279	0	TRP D	87	39.124	47.968	27.818	1.00	76.92
	5280	N	LEU D	88	40.465	46.386	28.690	1.00	86.84
	5281 5282	CA CB	LEU D	88	40.070	46.643	30.064	1.00	86.84
	5283	CG	LEU D	88	39.344	45.435	30.635	1.00	73.66
40	5284	CD1	LEU D	88 88	38.028 37.368	45.109	29.953	1.00	73.66
••	5285	CD2	LEU D	88	37.366 37.156	43.952 46.335	30.664	1.00	73.66
	5286	C	LEU D	88	41.248	46.962	29.991	1.00	73.66
	5287	ŏ	LEU D	88	42.330	46.396	30.953 30.820	1.00 1.00	86.84
	5288	Ň	LEU D	89	41.022	47.870	31.883	1.00	86.84
45	5289	CA	LEU D	89	42.067	48.266	32.809	1.00	45.19 45.19
	5290	CB	LEU D	89	42.573	49.655	32.473	1.00	158.38
	5291	CG	LEU D	89	43.628	50.105	33.471	1.00	158.38
	5292	CD1	LEU D	89	44.671	49.002	33.642	1.00	158.38
~~	5293	CD2	LEU D	89	44.255	51.392	32.982	1.00	158.38
50	5294	С	LEU D	89	41.502	48.263	34.219	1.00	45.19
	5295	0	LEU D	89	40.455	48.848	34.463	1.00	45,19
	5296	N	LEU D	90	42.164	47.592	35.153	1.00	80.53
	5297	CA	LEU D	90	41.666	47.579	36.523	1.00	80.53
55	5298	CB	LEU D	90	42.086	46.305	37.234	1.00	38.85
33	5299	CG	LEU D	90	41.710	46.256	38.724	1.00	38.85
	5300 5301	CD1	LEU D	90	40.189	46.295	38.793	1.00	38.85
	5302	CD2	LEU D	90	42.228	45.002	39.432	1.00	38.85
	5303	C	LEU D	90	42.245	48.766	37.280	1.00	80.53
60	5304	Ň	GLN D	90	43.445	48.858	37.467	1.00	80.53
00	5305	CA	GLN D	91	41.400	49.670	37.742	1.00	44.32
	5306	CB	GLN D	91 91	41.899	50.833	38.464	1.00	44.32
	5307	ca	GLN D	91	41.209 41.391	52.089 52.283	37.953	1.00	57.44
	5308	CD	GLN D	91	40.897		36.487	1.00	57.44
65	5309	OE1	GLN D	91	39.700	53.611 53.857	36.016 35.070	1.00	57.44
	5310	NE2	GLN D	91	41.816	53.657 54.489	35.979 35.664	1.00	57.44
	5311	C	GLN D	91	41.685	50.714	35.664 39.963	1.00	57.44
	5312	Õ	GLN D	91	40.691	50.176	40.435	1.00 1.00	44.32 44.32
	5313	N	ALA D	92	42.613	51.230	40.737	1.00	44.32 48.50
70	5314	CA	ALA D	92	42.451	51.152	42.169	1.00	48.50
						•			40.50

	5315	СВ	ALA D	92	43.463	50.199	42.739	1.00	52.70
	5316	Ç	ALA D	92	42.636	52.538	42.787	1.00	48.50
	5317	0 .	ALA D	92	43.475	53.347	42.341	1.00	48.50
5	5318 5319	N . CA	SER D SER D	93 93	41.846 41.960	52.825 54.102	43.811	1.00	53.99
_	5320	CB	SER D	93	41.048	54.102 54.158	44.481 45.713	1.00 1.00	53.99
	5321	ÖĞ	SER D	93	41.207	53.030	46.543	1.00	83.49 83.49
	5322	С	SER D	93	43.412	54.212	44.877	1.00	53.99
10	5323	0	SER D	93	44.134	55.046	44.361	1.00	53.99
10	5324	N OA	ALA D	94	43.850	53.338	45.764	1.00	62.76
	5325 5326	CA CB	ALA D ALA D	94 94	45.232	53.342	46.220	1.00	62.76
	5327	C	ALA D	94	45.301 45.723	53.851 51.909	47.636 46.150	1.00 1.00	112.27
	5328	ŏ	ALA D	94	44.942	50.990	46.361	1.00	62.76 62.76
15	5329	N	GLU D	95	47.006	51.704	45.854	1.00	73.31
	5330	CA	GLU D	95	47.535	50.339	45.746	1.00	73.31
	5331	CB	GLU D	95	48.677	50.301	44.746	1.00	116.96
	5332 5333	CG CL	GLU D	95 05	48.262	50.756	43.364	1.00	116.96
20	5334	OE1	GLU D	95 95	49.287 49.057	50.405 50.758	42.301 41.121	1.00	116.96
	5335	OE2	GLU D	95	50.320	49.776	42,643	1.00 1.00	116.96 116.96
	5336	С	GLU D	95	47.987	49.724	47.063	1.00	73.31
	5337	0	GLU D	95	48.194	48.517	47.143	1.00	73.31
25	5338	N	VAL D	96	48.139	50.563	48.089	1.00	71.30
23	5339 5340	CA CB	VAL D VAL D	96 96	48.557	50.126	49.422	1.00	71.30
	5341	CG1	VAL D	96 96	50.010 50.502	50.433 49.611	49.657	1.00	83.19
	5342	CG2	VAL D	96	50.802	50.132	50.812 48.410	1.00 1.00	83.19
	5343	c	VAL D	96	47.713	50.869	50.435	1.00	83.19 71.30
30	5344	0	VAL D	96	47.560	52.071	50.347	1.00	71.30
	5345	N	VAL D	97	47.190	50.159	51.420	1.00	69.41
	5346 5347	CA CB	VAL D	97	46.277	50.778	52.365	1.00	69.41
	5347 5348	CG1	VAL D VAL D	97 97	44.849 43.889	50.417 51.256	51.970 50.747	1.00	60.29
35	5349	CG2	VAL D	97	44.654	50.562	52.717 50.501	1.00 1.00	60.29 60.29
	5350	C	VAL D	97	46.410	50.374	53.828	1.00	69.41
	5351	0	VAL D	97	46.540	49.185	54.136	1.00	69.41
	5352	N	MET D	98	46.316	51.350	54.730	1.00	72.66
40	5353 5354	CA CB	MET D	98	46.389	51.084	56.169	1.00	72.66
40	5355	CG	MET D	98 98	46.498 47.751	52.404 53.177	56.921 56.594	1.00	249.19
	5356	SD	MET D	98	49.140	52.518	57.501	1.00 1.00	249.19 249.19
	5357	CE	MET D	98	48.761	53.180	59.122	1.00	249.19
45	5358	Č	MET D	98	45.110	50.363	56.592	1.00	72.66
45	5359	0	MET D	98	44.014	50.780	56.201	1.00	72.66
	5360 5361	N CA	GLU D	99	45.234	49.288	57.373	1.00	68,49
	5362	CB	GLU D	99 99	44.063 44.441	48.535 47.605	57.828 58.977	1.00 1.00	68.49
	5363	CG	GLU D	99	43.474	46.454	59.176	1.00	249.24 249.24
50	5364	CD	GLU D	99	43.683	45.744	60.499	1.00	249.24
	5365	OE1	GLU D	99	44.852	45.590	60.913	1.00	249.24
	5366	OE2	GLU D	99	42.679	45.331	61.120	1.00	249.24
	5367 5368	. C	GLU D	99	43.007	49.529	58.315	1.00	68.49
55	5369	Ň	GLY D	99 100	43.308 41.786	50.396 49.439	59.129 57.807	1.00	68.49
	5370	CA	GLY D	100	40.757	50.360	57.807 58.251	1.00 1.00	99.19 99.19
	5371	C	GLY D	100	40.336	51.428	57.256	1.00	99.19
	5372	0	GLY D	100	39.252	52.016	57.398	1.00	99.19
60	5373	N	GLN D	101	41.167	51.678	56.244	1.00	64.03
00	5374 5375	CA CB	GLN D GLN D	101	40.845	52.709	55.249	1.00	64.03
	5376	ca	GLN D	101 101	42.121 42.956	53.294 54.053	54.653	1.00	115.74
	5377	ČĎ	GLN D	101	42.145	55.055	55.650 56.435	1.00 1.00	115.74 115.74
	5378	OE1	GLN D	101	41.427	54.698	57.365	1.00	115.74
65	5379	NE2	GLN D	101	42.246	56.318	56.053	1.00	115.74
	5380	C	GLN D	101	39.939	52.240	54.118	1.00	64.03
	5381 5382	O N	GLN D PRO D	101	39.701	51.050	53.960	1.00	64.03
	5383	CD	PRO D	102 102	39.411 39.527	53.178 54.647	53.317	1.00	85.32
70	5384	CA	PRO D	102	38.536	54.647 52.761	53.374 52.218	1.00 1.00	90.00 85.32
						JE., J.	OE.E 10	1.00	00.32

	5385	СВ	PRO D	102	37.759	54.032	E4 044		
	5386	ČĠ	PRO D	102	38.814	54.032 55.078	51.911 52.098	1.00 1.00	90.00
	5387	C .	PRO D	102	39.365	52.273	51.026	1.00	85.32
5	5388 5389	0	PRO D	102	40.528	52.659	50.867	1.00	85.32
J	5390	N CA	LEU D	103 103	38.760 39.424	51.430 50.903	50.194	1.00	84.38
	5391	CB	LEU D	103	39.973	49.525	49.016 49.315	1.00 1.00	84.38
	5392	CG	LEU D	103	40.655	48.977	48.070	1.00	75.67 75.67
10	5393 5394	CD1	LEU D	103	41.849	49.845	47.739	1.00	75.67
10	5395	CD2 C	LEU D	103 103	41.095 38.467	47.543 50.792	48.305	1.00	75.67
	5396	ŏ	LEU D	103	37.453	50.135	47.854 47.974	1.00 1.00	84.38
	5397	N	PHE D	104	38.771	51.419	46.728	1.00	84.38 75.73
15	5398 5399	CA CB	PHE D	104	37.865	51.312	45.586	1.00	75.73
13	5400	CG	PHE D PHE D	104 104	37.272 36.530	52.679 53.359	45.208 46.322	1.00	163.52
	5401	CD1	PHE D	104	37.222	53.984	46.322 47.352	1.00 1.00	163.52 163.52
	5402	CD2	PHE D	104	35.139	53.381	46.342	1.00	163.52
20	5403 5404	CE1 CE2	PHE D	104	36.542	54.625	48.393	1.00	163.52
20	5405	CZ	PHE D PHE D	104 104	34.446 35.152	54.020 54.643	47.381	1.00	163.52
	5406	Č	PHE D	104	38.550	50.717	48.407 44.353	1.00 1.00	163.52
	5407	0	PHE D	104	39.617	51.181	43.942	1.00	75.73 75.73
25	5408	N	LEU D	105	37.950	49.684	43.769	1.00	46.40
23	5409 5410	CA CB	LEU D	105 105	38.504 38.633	49.069	42.561	1.00	46.40
	5411	CG	LEU D	105	39.461	47.555 47.169	42.7 <u>22</u> 43.932	1.00 1.00	51.89
	5412	CD1	LEU D	105	39.723	45.660	43.969	1.00	51.89 51.89
30	5413	CD2	LEU D	105	40.750	47.942	43.836	1.00	51.89
50	5414 5415	C O	LEU D	105 105	37.518 36.330	49.366	41.456	1.00	46.40
	5416	Ň	ARG D	106	37.988	49.413 49.551	41.701 40.236	1.00 1.00	46.40
	5417	CA	ARG D	106	37.073	49.852	39.159	1.00	68.20 68.20
35	5418	CB	ARG D	106	37.090	51.354	38.922	1.00	103.77
33	5419 5420	CG CD	ARG D ARG D	106 106	36.259 36.514	51.801	37.762	1.00	103.77
	5421	NE	ARG D	106	35.766	53.271 53.701	37.452 36 <i>.2</i> 75	1.00 1.00	103.77
	5422	CZ	ARG D	106	36.095	54.738	35.519	1.00	103.77 103.77
40	5423	NH1	ARG D	106	37.170	55.458	35.811	1.00	103.77
+0	5424 5425	NH2 C	ARG D ARG D	106 106	35.353 37.457	55.044	34.462	1.00	103.77
	5426	ŏ	ARG D	106	38.595	49.119 49.240	37.876 37.415	1.00 1.00	68.20
	5427	N	CYS D	107	36.535	48.340	37.309	1.00	68.20 54.86
45	5428	CA	CYS D	107	36.842	47.659	36.053	1.00	54.86
73	5429 5430	C	CYS D CYS D	107 107	36. 52 8 35.365	48.688	34.983	1.00	54.86
	5431	ČВ	CYS D	107	35.984	49.000 46.421	34.720 35.850	1.00 1.00	54.86
	5432	SG	CYS D	107	36.664	45.289	34.601	1.00	81.59 81.59
50	5433 5434	N CA	HIS D	108	37.578	49.236	34.384	1.00	77.64
50	5435	CA CB	HIS D HIS D	108 108	37.449 38.460	50.285	33.386	1.00	77.64
	5436	ČĞ	HIS D	108	38.301	51.352 52.573	33.687 32.853	1.00 1.00	84.93
	5437	CD2	HIS D	108	39.176	53.230	32.060	1.00	84.93 84.93
55	5438	ND1	HIS D	108	37.136	53.301	32.834	1.00	84.93
<i>J</i>	5439 5440	CE1 NE2	HIS D HIS D	108	37.306	54.364	32.068	1.00	84.93
	5441	C	HIS D	108 108	38.534 37.608	54.346 49.848	31.587 31.945	1.00 1.00	84.93
	5442	0	HIS D	108	38.604	49.229	31.559	1.00	77.64 77.64
60	5443 5444	N	GLY D	109	36.618	50.206	31.143	1.00	64.08
00	5445	CA C	GLY D	109 109	36.637 37.367	49.820	29.750	1.00	64.08
	5446	ŏ	GLY D	109	37.498	50.854 52.002	28.945 29.379	1.00 1.00	64.08
	5447	Ŋ	TRP D	110	37.858	50.446	27.781	1.00	64.08 110.56
65	5448 5449	CA CB	TRP D	110	38.575	51.353	26.906	1.00	110.56
05	5450	CB CG	TRP D	110 110	39.206	50.578 E1.456	25.749	1.00	129.78
	5451	CD2	TRP D	110	39.819 41.184	51.456 51.879	24.721 24.659	1.00	129.78
	5452	CE2	TRP D	110	41.307	52.743	24.059 23.557	1.00 1.00	129.78 129.78
70	5453	CE3	TRP D	110	42.322	51.608	25.434	1.00	129.78
10	5454	CD1	TRP D	110	39.184	52.062	23.682	1.00	129.78

	5455	NE1	TRP D	110 -	40.068	52.836	22.977	4.00	400
	5456	CZ2	TRP D	110	42.514	53.345	23.204	1.00 1.00	129.78
	5457	CZ3	TRP D	110	43.525	52.208	25.083	1.00	129.78 129.78
_	5458	CH2	TRP D	110	43.609	53.068	23.980	1.00	129.78
5	5459	С	TRP D	110	37.623	52.414	26.377	1.00	110.56
	5460	0	TRP D	110	36.417	52.183	26.252	1.00	110.56
	5461	N	ARG D	111	38.170	53.591	26.091	1.00	110.12
	5462	CA	ARG D	111	37.377	54.696	25.564	1.00	110.12
10	5463 5464	CB	ARG D	111	37.068	54.455	24.113	1.00	249.23
10	5465	CG CD	ARG D	111	38.127	54.981	23.233	1.00	249.23
	5466	NE NE	ARG D	111 111	37.639 38.039	54.963	21.844	1.00	249.23
	5467	CZ	ARG D	111	37.564	56.180 57.390	21.160 21.444	1.00	249.23
	5468	NH1	ARG D	111	36.661	57.561	22.411	1.00 1.00	249.23
15	5469	NH2	ARG D	111	38.007	58,437	20.760	1.00	249.23 249.23
	5470	С	ARG D	111	36.070	54.939	26.286	1.00	110.12
	5471	0	ARG D	111	35.117	55.496	25.736	1.00	110.12
	5472	N _.	ASN D	112	36.031	54.502	27.527	1.00	80.55
20	5473	CA	ASN D	112	34.859	54.663	28.349	1.00	80.55
20	5474	CB	ASN D	112	34.546	56.137	28.546	1.00	69.20
	5475 5476	CG OD1	ASN D ASN D	112	33.765	56.379	29.815	1.00	69.20
	5477	ND2	ASN D	112 112	33.075	55.484	30.307	1.00	69.20
	5478	C		. 112	33.863 33.621	57.586 53.963	30.355	1.00	69.20
25	5479	ŏ	ASN D	112	32.500	54.357	27.813 28.143	1.00	80.55
	5480	Ň	TRP D	113	33.5↓-	52.930	26.998	1.00 1.00	80.55
	5481	CA	TRP D	113	32.649	52.207	26.504	1.00	104.63 104.63
	5482	CB	TRP D	113	33.045	51.128	25.519	1.00	141.29
20	5483	CG	TRP D	113	33.355	51.652	24.198	1.00	141.29
30	5484	CD2	TRP D	113	34.368	51.180	23.311	1.00	141.29
	5485	CE2	TRP D	113	34.278	51.944	22.133	1.00	141.29
	5486	CE3	TRP D	113	35.343	50.182	⁻ 23.397	1.00	141.29
	5487 5488	CD1 NE1	TRP D	113	32.705	52.655	23.541	1.00	141.29
35	5489	CZ2	TRP D	113 113	33.254 35.126	52.837 51.743	22.296	1.00	141.29
-	5490	CZ3	TRP D	113	36.188	51.743 49.984	21.057 22.324	1.00	141.29
	5491	CH2	TRP D	113	36.075	50.761	21.173	1.00 1.00	141.29
	5492	C	TRP D	113	31.928	51.542	27.656	1.00	141.29 104.63
40	5493	0	TRP D	113	32.215	51.806	28.828	1.00	104.63
40	5494	N	ASP D	114	30.990	50.668	27.313	1.00	117.64
	5495	CA	ASP D	114	30.229	49.960	28.320	1.00	117.64
	5496	CB	ASP D	114	28.725	50.109	28.065	1.00	192.42
	5497 5498	CG OD1	ASP D	114	28.176	51.431	28.576	1.00	192.42
45	5499	OD2	ASP D	114 114	28.288 27.636	51.685	29.796	1.00	192.42
15	5500	C	ASP D	114	30.619	52.214 48.498	27.764	1.00	192.42
	5501	ŏ	ASP D	114	30.831	47.875	28.345 27.301	1.00 1.00	117.64
	5502	Ñ	VAL D	115	30.730	47.967	29.559	1.00	117.64 73.71
	5503	CA	VAL D	115	31.084	46.577	29.766	1.00	73.71
50	5504	CB	VAL D	115	32.340	46.448	30.614	1.00	75.80
	5505	CG1	VAL D	115	32.827	45.011	30.593	1.00	75.80
	5506	CG2	VAL D	115	33.403	47.378	30.086	1.00	75.80
	5507 5508	C	VAL D	115	29.947	45.862	30.481	1.00	73.71
55	5509	O N	VAL D TYR D	115	29.301	46.431	31.368	1.00	73.7 1
55	5510	ČA .	TYR D	116 116	29.700 28.642	44.615 43.810	30.078	1.00	69.51
	5511	CB	TYR D	116	27.563	43.539	30.672 29.638	1.00	69.51
	5512	CG	TYR D	116	26.886	44.780	29.133	1.00 1.00	100.20 100.20
	5513	CD1	TYR D	116	27.276	45.376	27.942	1.00	100.20
60	5514	CE1	TYR D	116	26.660	48.549	27.481	1.00	100.20
	5515	CD2	TYR D	116	25.866	45.375	29.858	1.00	100.20
	5516	CE2	TYR D	116	25.243	46.545	29.412	1.00	100.20
	5517	CZ	TYR D	116	25.648	47.127	28.225	1.00	100.20
65	5518 5510	ОН	TYR D	116	25.060	48.293	27.795	1.00	100.20
U)	5519 5520	CO	TYR D	116	29.179	42.488	31.222	1.00	69.51
	5520 5521	N	TYR D LYS D	116	30.341	42.127	30.986	1.00	69.51
	5522	CA CA	LYS D	117 117	28.327 28.708	41.766 40.492	31.947	1.00	88.92
	5523	CB	LYS D	117	28.772	40.492 39.397	32.541 31.480	1.00 1.00	88.92
70	5524	CG	LYS D	117	27.453	38.715	31.180	1.00	111.93 111.93
									1:1.30

	5525	CD	LYS D	117	27.695	37.387	30.471	1.00	111.93
	5526	CE	LYS D	117	28.540	36.435	31.338	1.00	
	5527	NZ	LYS D	117	28.852	35.125	30.675		111.93
	5528	Ċ.	LYS D	117	30.069	40.625		1.00	111.93
5	5529	ŏ	LYS D	117	31.002		33.213	1.00	88.92
•	5530	Ň	VAL D			39.882	32.909	1.00	88.92
	5531			118	30.182	41.578	34.129	1.00	81.88
		CA	VAL D	118	31.433	41.816	34.828	1.00	81.88
	5532	CB	VAL D	118	31.524	43.274	35.241	1.00	84.78
10	5533	CG1	VAL D	118	32.404	43.434	36.459	1.00	84.78
10	5534	CG2	VAL D	118	32.104	44.055	34.101	1.00	84.78
	5535	С	VAL D	118	31.693	40.949	36.052	1.00	
	5536	0	VAL D	118	30.803	40.742	36.893	1.00	81.88
	5537	N	ILE D	119	32.928	40.468	36.171		81.88
	5538	CA	ILE D	119	33.296	39.637		1.00	56.52
15	5539	CB	ILE D				37.310	1.00	56.52
10	5540	CG2		119	33.364	38.181	36.895	1.00	59.73
			ILE D	119	33.652	37.309	38.094	1.00	59.73
	5541	CG1	ILE D	119	32.058	37.776	36.217	1.00	59.73
	5542	CD1	ILE D	119	32.154	36.446	35. 53 4	1.00	59.73
00	5543	С	ILE D	119	34.662	40.027	37.826	1.00	56.52
20	5544	0	ILE D	119	35.611	40.026	37.057	1.00	56.52
	5545	N	TYR D	120	34.785	40.378	39.104	1.00	
	5546	CA	TYR D	120	36.115	40.736	39.618	1.00	51.66
	5547	СВ	TYR D	120	36.064	41.770	40.742		51.66
	5548	ĊĠ	TYR D	120	35.658	43.139		1.00	57.63
25	5549	CD1	TYR D				40.320	1.00	57.63
	5550	CE1		120	34.336	43.470	40.170	1.00	57.63
			TYR D	120	33.960	44.720	39.744	1.00	57.63
	5551	CD2	TYR D	120	36.599	44.093	40.038	1.00	57.63
	5552	CE2	TYR D	120	36.237	45.353	39.609	1.00	57.63
20	5553	CZ	TYR D	120	34.915	45.656	39.464	1.00	57.63
30	5554	OH	TYR D	120	34.549	46.902	39.039	1.00	57.63
	5555	С	TYR D	120	36.702	39.486	40.200	1.00	51.66
	5556	0	TYR D	120	35.971	38.657	40.725	1.00	
	5557	Ň	TYR D	121	38.015	39.353	40.123		51.66
	5558	. CA	TYR D	121	38.667	38.180		1.00	46.59
35	5559	CB	TYR D	121	39.304		40.684	1.00	46.59
-	5560	CG				37.344	39.572	1.00	81.03
	5561	CD1	TYR D	121	38.357	36.640	38.623	1.00	81.03
			TYR D	121	37.541	37.362	37.761	1.00	81.03
	5562	CE1	TYR D	121	36.705	36.721	36.856	1.00	81.03
40	5563	CD2	TYR D	121	38.311	35.244	38.562	1.00	81.03
40	5564	CE2	TYR D	121	37.478	34.597	37.666	1.00	81.03
	5565	CZ	TYR D	121	36.672	35.345	36.808	1.00	81.03
	5566	OH	TYR D	121	35.835	34.720	35.894	1.00	81.03
	5567	С	TYR D	121	39.771	38.566	41.683	1.00	46.59
	5568	0	TYR D	121	40.518	39.538	41.473	1.00	46.59
45	5569	N	LYS D	122	39.876	37.809	42.770	1.00	72.20
	5570	CA	LYS D	122	40.920	38.054	43.759	1.00	
	5571	CB	LYS D	122	40.357	38.585	45.073		72.20
	5572	ČĠ	LYS D	122	41.440			1.00	128.16
	5573	CD	LYS D			38.842	46.100	1.00	128.16
50	5574	CE		122	40.869	39.066	47.470	1.00	128.16
50			LYS D	122	41.973	39.176	48. 49 6	1.00	128.16
	5575	NZ	LYS D	122	41.394	39.233	49.865	1.00	128.16
	5576	Ç	LYS D	122	41.598	36.736	44.028	1.00	72.20
	5577	0	LYS D	122	40.977	35.813	44.536	1.00	72.20
	5578	N	ASP D	123	42.876	36.658	43.692	1.00	101.46
55	5579	CA	ASP D	123	43.660	35.450	43.884	1.00	101.46
	5580	CB	ASP D	123	43.802	35.135	45.375	1.00	177.22
	5581	CG	ASP D	123	44.795	36.049	46.065	1.00	
	5582	OD1	ASP D	123	45.903	36.238			177.22
	5583	OD2	ASP D	123			45.518	1.00	177.22
60	5584	Č	ASP D		44.477	36.572	47.154	1.00	177.22
••	5585	ŏ		123	43.079	34.258	43.138	1.00	101.46
			ASP D	123	43.017	33.147	43.668	1.00	101.46
	5586	N	GLY D	124	42.661	34.502	41.898	1.00	89.52
	5587	CA	GLY D	124	42.103	33.456	41.056	1.00	89.52
66	5588	Ç	GLY D	124	40.673	33.041	41.346	1.00	89.52
65	5589	0	GLY D	124	40.092	32.261	40.587	1.00	89.52
	5590	N	GLU D	125	40.097	33.559	42.428	1.00	72.85
	5591	CA	GLU D	125	38.730	33.206	42.826		
	5592	CB	GLU D	125	38.599	33.194		1.00	72.85
	5593	CG	GLU D	125			44.362	1.00	232.74
70	5594	CD	GLU D	125	39.348	32.082	45.103	1.00	232.74
. •		Ju	GLO D	123	38.625	30.746	45.068	1.00	232.74
						•			

	5595	OE1	GLU D	125	37.493	30.662	45.593	1.00	232.74
	5596	OE2	GLU D	125	39.194	29.780	44.517	1.00	232.74
	5597 5598	С О .	GLU D	125	37.706	34.202	42.280	1.00	72.85
5	5599	N	GLU D	125	37.974	35.404	42.183	1.00	72.85
,	5600	CA	ALA D ALA D	126 126	36.527	33.708	41.926	1.00	95.10
	5601	CB	ALA D	126	35.472 34.290	34.595 33.791	41.450	1.00	95.10
	5602	C	ALA D	126	35.119	35.403	40.991	1.00	132.03
	5603	ŏ	ALA D	126	35.153	34.869	42.693 43.802	1.00	95.10
10	5604	Ň	LEU D	127	34.782	36.678	43.502	1.00 1.00	95.10
	5605	CA	LEU D	127	34.470	37.522	43.697	1.00	64.20
	5606	СВ	LEU D	127	35.559	38.566	43.919	1.00	64.20 89.10
	5607	CG	LEU D	127	35.546	38.957	15.392	1.00	89.10
1 =	5608	CD1	LEU D	127	35.768	37.691	46.219	1.00	89.10
15	5609	CD2	LEU D	127	36.612	39.988	+5.686	1.00	89.10
	5610	C	LEU D	127	33.138	38.237	43.722	1.00	64.20
	5611	0 N	LEU D	127	32.408	38.098	44.686	1.00	64.20
	5612 5613	CA	LYS D LYS D	128	32.859	39.041	42.702	1.00	63.83
20	5614	CB	LYS D	128 128	31.584	39.742	42.583	1.00	63.83
	5615	CG	LYS D	128	31.737 32.165	41.203	43.000	1.00	126.01
	5616	CD	LYS D	128	31.058	41.409 41.080	44.431	1.00	126.01
	5617	CE	LYS D	128	31.491	41.410	45.416 46.843	1.00	126.01
_	5618	NZ	LYS D	128	30.404	41.252	47.855	1.00 1.00	126.01
25	5619	C	LYS D	128	31.160	39.675	41.109	1.00	126.01 63.83
	5620	0	LYS D	128	32.021	39.580	40.219	1.00	63.83
	5621	N	TYR D	129	29.857	39.741	40.833	1.00	62.64
	5622	CA	TYR D	129	29.387	39.683	39.444	1.00	62.64
30	5623	CB	TYR D	129	28.984	38.268	39.098	1.00	80.75
30	5624	CG	TYR D	129	28.046	38.200	37.928	1.00	80.75
	5625 5626	CD1 CE1	TYR D	129	28.521	38.321	36.629	1.00	80.75
	5627	CD2	TYR D TYR D	129	27.652	38.296	35.533	1.00	80.75
	5628	CE2	TYR D	129 129	26.682 25.803	38.057	38.118	1.00	80.75
35	5629	CZ	TYR D	129	26.288	38.042 38.160	37.037	1.00	80.75
	5630	ОH	TYR D	129	25.412	38.145	35.741 34.662	1.00	80.75
	5631	Č	TYR D	129	28.192	40.564	39.182	1.00 1.00	80.75
	5632	0	TYR D	129	27.268	40.602	39.996	1.00	62.64 62.64
40	5633	N	TRP D	130	28.190	41.252	38.042	1.00	93.45
40	5634	CA	TRP D	130	27.076	42.123	37.680	1.00	93.45
	5635	CB	TRP D	130	27.356	43.561	38.092	1.00	113.53
	5636	CG	TRP D	130	27.799	43.749	39.506	1.00	113.53
	5637 5638	CD2 CE2	TRP D	130	27.020	44.284	40.583	1.00	113.53
45	5639	CE3	TRP D	130	27.863	44.336	41.718	1.00	113.53
	5640	CD1	TRP D	130 130	25.690 29.043	44.716	40.700	1.00	113.53
	5641	NE1	TRP D	130	29.092	43.512 43.864	40.018 41.347	1.00	113.53
	5642	CZ2	TRP D	130	27.413	44.811	42.961	1.00	113.53
	5643	CZ3	TRP D	130	25.242	45.191	41.945	1.00 1.00	113.53
50	5644	CH2	TRP D	130	26.104	45.238	43.051	1.00	113.53 113.53
	5645	С	TRP D	130	26.817	42.119	36.181	1.00	93.45
	5646	0	TRP D	130	27.643	41.649	35.404	1.00	93.45
	5647	N	TYR D	131	25.667	42.650	35.773	1.00	68.85
55	5648	CA	TYR D	131	25.343	42.732	34.351	1.00	68.85
23	5649	CB	TYR D	131	23.835	42.746	34.119	1.00	129.65
	5650 5651	CG CD1	TYR D	131	23.515	42.570	32.657	1.00	129.65
	5652	CE1	TYR D	131	23.660	41.330	32.046	1.00	129.65
	5653	CD2	TYR D	131 131	23.494	41.183	30.685	1.00	129.65
60	5654	CE2	TYR D	131	23.182 23.015	43.661 43.523	31.862	1.00	129.65
	5655	CZ	TYR D	131	23.177	42.282	30.495	1.00	129.65
	5656	OH	TYR D	131	23.056	42.154	29.915 28.555	1.00 1.00	129.65 129.65
	5657	С	TYR D	131	25.953	44.035	33.846	1.00	68.85
~ =	5658	0	TYR D	131	27.035	44.028	33.249	1.00	68.85
65	5659	N _.	GLU D	132	25.234	45.142	34.045	1.00	110.47
	5660	CA	GLU D	132	25.761	46.455	33.684	1.00	110.47
	5661	CB	GLU D	132	24.715	47.569	33.878	1.00	169.41
	5662	CG	GLU D	132	23.632	47.688	32.798	1.00	169.41
70	5663 5664	CD OE1	GLU D	132	23.679	49.022	32.059	1.00	169.41
, ,	3004	JET	GLU D	132	24.276	49.981	32.594	1.00	169.41

	ECCE	OEO	0	455					
	5665 5666	OE2 C	GLU D GLU D	132 132	23.107 26.765	49.114 46.491	30.951	1.00	169.41
	5667	ŏ	GLU D	132	26.391	46.249	34.814 35.965	1.00 1.00	110.47
_	5668	Ν.	ASN D	133	28.029	46.777	34.515	1.00	110.47 115.67
5	5669	CA	ASN D	133	29.030	46.736	35.574	1.00	115.67
	5670 5671	CB CG	ASN D ASN D	133 133	30.448	46.807	35.003	1.00	113.79
	5672	OD1	ASN D	133	30.911 30.200	48.198 49.009	34.814 34.233	1.00	113.79
	5673	ND2	ASN D	133	32.110	48.501	35.296	1.00 1.00	113.79
10	5674	С	ASN D	133	28.888	47.723	36.718	1.00	113.79 115.67
	5675	0	ASN D	133	28.054	48.618	36.717	1.00	115.67
	5676 5677	N CA	HIS D HIS D	134 134	29.747	47.518	37.702	1.00	133.45
	5678	CB	HIS D	134	29.748 29.100	48.283 47.430	38.921 40.006	1.00	133.45
15	5679	CG	HIS D	134	28.893	48.141	41.302	1.00 1.00	207.58 207.58
	5680	CD2	HIS D	134	29.411	47.919	42.534	1.00	207.58
	5681	ND1	HIS D	134	28.039	49.213	41.435	1.00	207.58
	5682 5683	CE1 NE2	HIS D HIS D	134 134	28.038 28.862	49.620	42.690	1.00	207.58
20	5684	C	HIS D	134	31.188	48.851 48.609	43.378 39.290	1.00 1.00	207.58
	5685	0	HIS D	134	32.091	48.473	38.469	1.00	133.45 133.45
	5686	N	ASN D	135	31.388	49.015	40.537	1.00	73.71
	5687 5688	CA CB	ASN D	135	32.701	49.394	41.017	1.00	73.71
25	5689	CG	ASN D ASN D	135 135	32.877 32.913	50.923 51.402	40.922	1.00	127.04
	5690	OD1	ASN D	135	33.606	50.790	39.490 38.668	1.00 1.00	127.04
	5691	ND2	ASN D	135	32.193	52.478	39.170	1.00	127.04 127.04
	5692	C	ASN D	135	32.869	48.930	42.441	1.00	73.71
30	5693 5694	0 N	ASN D ILE D	135	32.604	49.672	43.363	1.00	73.71
50	5695	CA	ILE D	136 136	33.307 33.534	47.689 47.094	42.606 43.918	1.00 1.00	72.93
	5696	CB	ILE D	136	34.435	45.852	43.786	1.00	72.93 89.30
	5697	CG2	ILE D	136	35.652	46.164	42.961	1.00	89.30
35	5698 5699	CG1 CD1	ILE D	136	34.828	45.348	45.159	1.00	89.30
55	5700	CDI	ILE D	136 136	35.595 34.139	44.057 48.097	45.088	1.00	89.30
	5701	ŏ	ILE D	136	35.241	48.602	44.892 44.689	1.00 1.00	72.93
	5702	N	SER D	137	33.393	48.393	45.952	1.00	72.93 72.75
40	5703	CA	SER D	137	33.810	49.378	46.952	1.00	72.75
40	5704 5705	CB OG	SER D SER D	137 137	32.797	50.514	46.982	1.00	69.16
	5706	Č	SER D	137	32.966 33.965	51.300 48.811	48.135 48.356	1.00 1.00	69.16
	5707	0	SER D	137	33.227	47.922	48.765	1.00	72.75 72.75
45	5708	N	ILE D	138	34.914	49.348	49.106	1.00	112.14
43	5709 5710	CA CB	ILE D	138	35.171	48.888	50.464	1.00	112.14
	5710 5711	CG2	ILE D	138 138	36.436 36.827	48.063 47.824	50.515	1.00	65.89
	5712	CG1	ILE D	138	36.239	46.759	51.962 49.745	1.00 1.00	65.89 65.89
50	5713	CD1	ILE D	138	37.523	46.004	49.492	1.00	65.89
50	5714	C	ILE D	138	35.359	50.050	51.431	1.00	112.14
	5715 5716	O N	ILE D THR D	138 139	36.253	50.879	51.244	1.00	112.14
	5717	CA CA	THR D	139	34.544 34.628	50.092 51.172	52.483 53.464	1.00	70.90
	5718	CB	THR D	139	33.330	51.276	54. 253	1.00 1.00	70.90 212.07
55	5719	OG1	THR D	139	32.988	49.984	54.771	1.00	212.07
	5720 5721	CG2	באני ס	139	32.212	51.772	53.352	1.00	212.07
	5721 5722	C	THR D THR D	139 139	35.791	50.913	54.409	1.00	70.90
	5723	Ň	ASN D	140	36.851 35.586	51.523 50.005	54.280 55.356	1.00	70.90
60	5724	CA	ASN D	140	36.606	49.640	56.333	1.00 1.00	80.70 80.70
	5725	CB	ASN D	140	35.957	49.206	57.644	1.00	232.63
	5726 5727	CG OD1	ASN D	140	36.967	48.690	58.636	1.00	232.63
	5728	ND2	ASN D ASN D	140 140	37.818 36.862	47.864	58.318	1.00	232.63
65	5729	C	ASN D	140	37.344	49.170 48.464	59.865 55.709	1.00 1.00	232.63
	5730	0	ASN D	140	36.732	47.447	55.411	1.00	80.70 80.70
	5731	N	ALA D	141	38.650	48.593	55.503	1.00	77.89
	5732 5733	CA CB	ALA D	141	39.428	47.522	54.870	1.00	77.89
70	5734	C	ALA D ALA D	141 141	40.437 40.142	48.086 46.600	53.919	1.00	47.27
-		-	,		TV. 174	46.600	55.822	1.00	77.89

10 14 14 14 14 15 14 15 15		5735 5736	O N	ALA D	141	40.885	47.017	56.703	1.00	77.89
5738 CB THR D 142 39.346 43.343 56.442 1.00 18.80 5740 CG2 THR D 142 39.346 43.343 56.745 1.00 18.80 5741 C THR D 142 49.274 44.055 55.837 1.00 73.00 18.80 5741 C THR D 142 49.274 44.055 55.837 1.00 73.00 18.80 5742 O THR D 142 49.273 44.055 55.837 1.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.00 73.0		5736 5737		THR D	142	39.941	45.317	55.606	1.00	73.90
5 5739 OQ1 THR D 142 38.346 43.343 56.245 1.00 198.80 5746 CQ2 THR D 142 40.214 42.014 57.416 1.00 198.80 5741 C THR D 142 42.236 44.055 55.837 1.00 198.80 5741 C THR D 142 42.236 44.055 55.837 1.00 198.80 5742 O THR D 142 42.236 44.056 54.779 1.00 73.90 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.50 19.										
5740 CG2 THR D 142 40.214 42.014 57.416 1.00 193.80 5746 5741 C THR D 142 41.927 44.055 55.8377 1.00 178.80 5742 O THR D 142 41.2276 44.506 55.55.377 1.00 178.80 5742 O THR D 142 42.236 44.506 55.55.377 1.00 178.80 5743 N VAL D 143 42.756 43.288 56.521 1.00 104.07 5745 CB VAL D 143 44.088 42.953 56.008 1.00 104.07 5745 CB VAL D 143 44.088 42.953 56.008 1.00 104.07 5745 CB VAL D 143 44.084 42.953 56.008 1.00 104.07 5745 CB VAL D 143 44.084 47.01 41.320 57.807 1.00 127.52 5746 CC VAL D 143 44.701 41.320 57.807 1.00 127.52 5746 CC VAL D 143 44.701 41.320 57.807 1.00 127.52 5746 CC VAL D 143 44.985 42.479 55.545 1.00 127.52 5746 CC VAL D 143 44.986 42.479 55.545 1.00 127.52 5746 CC VAL D 143 44.869 42.479 55.545 1.00 127.52 5746 CC VAL D 143 44.869 41.764 55.107 1.00 104.07 5759 CG GG GLU D 144 42.822 41.046 55.222 1.00 67.28 5751 CG GG GLU D 144 41.840 33.915 51.00 57.28 5753 CG GG GLU D 144 41.840 39.243 39.814 54.000 1.00 87.28 5753 CG GG GLU D 144 41.840 39.768 39.428 55.033 1.00 215.80 5755 CC GLU D 144 41.840 39.756 38.856 57.409 1.00 215.80 5756 CE GLU D 144 41.840 39.756 38.856 57.409 1.00 215.80 5756 CE GLU D 144 41.840 39.756 38.856 57.409 1.00 215.80 5756 CE GLU D 144 41.840 39.756 38.856 57.409 1.00 215.80 5756 CE GLU D 144 41.840 39.756 38.856 57.409 1.00 215.80 5756 CE GLU D 144 41.840 39.756 38.856 57.409 1.00 215.80 5756 CE GLU D 144 42.245 40.287 52.982 1.00 215.80 5756 CE GLU D 144 41.840 39.756 38.856 57.409 1.00 215.80 5756 CE GLU D 144 41.840 39.756 38.856 57.409 1.00 215.80 5756 CE GLU D 144 42.245 40.847 59.592 1.00 215.80 5756 CE GLU D 144 41.840 39.756 59.982 1.00 215.80 5756 CE GLU D 144 42.245 40.847 59.592 1.00 215.80 5756 CE GLU D 144 42.245 40.847 59.592 1.00 215.80 5756 CE GLU D 144 42.245 40.847 59.592 1.00 215.80 5756 CE GLU D 144 42.245 40.847 59.592 1.00 215.80 5756 CE GLU D 144 42.245 40.847 59.592 1.00 215.80 5756 CE GLU D 144 42.245 40.847 59.592 1.00 215.80 5756 CE GLU D 144 42.245 40.847 59.592 1.00 215.80 5756 CE GLU D 144 54.840 54.840 54.840 55.500 57.60 57.60 5756 CE GLU	5									
5741 C THR D 142 4228 41.927 44.055 55.837 1.00 73.80 5745 N VAL D 142 42.276 44.055 55.837 1.00 73.80 5746 C N VAL D 143 42.756 43.268 55.211 1.00 70.407 5746 C B VAL D 143 45.093 42.610 57.127 1.00 104.07 5746 C G1 VAL D 143 45.093 42.610 57.127 1.00 127.52 5747 C G2 VAL D 143 44.098 42.955 56.008 1.00 104.07 57546 C G1 VAL D 143 44.093 57.127 1.00 127.52 5747 C G2 VAL D 143 48.095 42.479 55.545 1.00 127.52 5748 C O VAL D 143 48.095 41.736 55.107 1.00 127.52 5758 C A GLU D 144 42.603 39.011 55.003 1.00 27.28 5751 C A GLU D 144 42.603 39.011 55.003 1.00 67.28 5752 C B GLU D 144 42.603 39.011 55.003 1.00 27.58 5756 O C GLU D 144 42.893 39.015 55.381 1.00 215.80 5757 C C GLU D 144 42.283 39.016 57.477 1.00 215.80 5758 O C GLU D 144 42.283 39.016 57.477 1.00 215.80 5759 N G GLU D 144 42.283 39.016 57.477 1.00 215.80 5756 O C GLU D 144 42.283 39.016 57.409 1.00 215.80 5757 C C G GLU D 144 42.283 39.016 57.409 1.00 215.80 5758 O C GLU D 144 42.283 39.016 57.409 1.00 215.80 5758 O C GLU D 144 42.283 39.478 55.007 1.00 215.80 5758 O C GLU D 144 42.283 39.478 55.007 1.00 215.80 5759 N ASP D 145 39.488 34.283 55.2074 1.00 215.80 5760 C A ASP D 145 39.488 34.283 55.2074 1.00 215.80 5760 C A ASP D 145 39.488 34.283 55.2074 1.00 27.28 5760 C A SP D 145 39.488 34.283 55.2074 1.00 27.24 5765 C C A SP D 145 39.488 34.283 55.2074 1.00 27.24 5766 O ASP D 145 39.488 34.320 52.163 1.00 22.84 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5766 C A SP D 145 39.488 42.295 49.365 1.00 22.33 5767 C C G G F C G G G G G G G G G G G G G G	•									
5742										
10 5744		5742	0							
10 5744	••				143	42.756	43.268			
5746 CBI VAL D 143 44.701 41.320 57.807 1.00 127.52 5747 CG2 VAL D 143 44.701 41.320 57.807 1.00 127.52 5748 C VAL D 143 44.985 42.479 56.545 1.00 127.52 5748 C VAL D 143 44.985 42.479 56.545 1.00 104.07 5750 N GU D 143 42.829 11.046 55.222 1.00 104.07 5750 N GU D 144 42.829 11.046 55.222 1.00 67.28 5751 CA GUU D 144 42.829 11.046 55.222 1.00 67.28 5752 CB GU D 144 41.849 39.011 55.003 1.00 215.80 5753 CB GU D 144 41.849 39.011 55.003 1.00 215.80 5754 CD GU D 144 41.849 39.001 57.475 1.00 215.80 5756 CC GUU D 144 41.855 39.506 58.416 1.00 215.80 5756 CC GUU D 144 42.288 39.478 52.074 1.00 67.28 5758 C G GU D 144 42.288 39.478 52.074 1.00 67.28 5759 C G GU D 144 42.288 39.478 52.074 1.00 67.28 5750 CA ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5763 C G ASP D 145 40.847 41.848 41.8320 52.163 1.00 129.44 5765 C G ASP D 145 40.847 41.848 41.8320 52.163 1.00 129.44 5768 C G ASP D 145 40.847 41.848 41.8320 52.163 1.00 129.44 5768 C G ASP D 146 42.634 42.634 42.636 51.510 1.00 129.44 5768 C G ASP D 146 42.734 42.737 43.448 41.00 42.235 51.00 67.03 5769 C G ASP D 146 40.848 41.832 42.636 51.510 1.00 129.44 5768 C G C G G G G G G G G G G G G G G G G	10							56.008	1.00	
5747										127.52
5748										
15 5749 O VAL D 143 44 846 41 424 54 322 1 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 1										
5750 N GLU D 144 42.829 41.046 55.222 1.00 67.28 5751 CA GLU D 144 42.803 38.74 54.400 1.00 67.28 5752 C8 GLU D 144 41.492 33.011 55.003 1.00 215.80 5753 CG GLU D 144 41.492 33.011 55.003 1.00 215.80 5755 CD GLU D 144 41.840 33.021 55.003 1.00 215.80 5755 CD GLU D 144 41.855 33.855 57.409 1.00 215.80 5756 OE2 GLU D 144 41.555 33.855 57.409 1.00 215.80 5756 OE2 GLU D 144 41.555 33.855 57.409 1.00 215.80 5756 OE2 GLU D 144 41.555 33.856 57.409 1.00 215.80 5758 OE3	15									
5751 CA GLU D 144 42.603 39.874 54.400 1.00 87.28 5752 CB GLU D 144 41.492 39.011 55.003 1.00 215.80 5753 CG GLU D 144 41.492 39.011 55.003 1.00 215.80 5755 OE1 GLU D 144 41.840 39.23 90.01 57.475 1.00 215.80 5756 OE2 GLU D 144 39.756 38.856 57.409 1.00 215.80 5757 C GLU D 144 42.245 39.596 54.16 1.00 215.80 5757 C GLU D 144 42.245 40.287 52.982 1.00 87.28 5758 O GLU D 144 42.245 40.287 52.982 1.00 87.28 5758 O GLU D 144 42.245 40.287 52.982 1.00 87.28 5758 O GLU D 144 42.248 39.478 52.074 1.00 87.28 5758 O GLU D 144 42.248 39.478 52.074 1.00 87.28 5758 C G ASP D 145 40.847 43.441 51.634 1.00 129.44 5763 OD1 ASP D 145 39.484 43.320 52.163 1.00 129.44 5765 C G ASP D 145 39.484 43.320 52.163 1.00 129.44 5765 C ASP D 145 39.158 43.899 53.228 1.00 129.44 5766 O ASP D 145 39.484 43.320 52.163 1.00 129.44 5766 O ASP D 145 39.484 43.320 52.163 1.00 129.44 5766 O ASP D 145 43.894 42.235 50.383 1.00 89.85 5760 CA SER D 146 43.892 42.217 50.587 1.00 67.03 5760 CA SER D 146 43.892 42.217 50.587 1.00 67.03 5760 CA SER D 146 43.892 42.217 50.587 1.00 67.03 5760 CA SER D 146 43.892 42.217 51.100 67.03 5760 CA SER D 146 43.892 42.217 51.00 67.03 5770 OG SER D 146 43.892 42.217 51.00 67.03 5770 OG SER D 146 43.892 42.217 51.00 67.03 5770 OG SER D 146 43.892 42.217 51.00 67.51 5777 N GLY D 149 44.800 40.693 48.865 1.00 67.51 5777 N G SER D 146 44.810 39.333 49.836 1.00 89.85 5770 O SER D 146 43.86 42.777 1.00 69.85 5770 O SER D 146 43.76 39.898 44.835 1.00 67.51 5776 C G LY D 147 45.694 41.255 44.800 1.00 67.51 5776 C G LY D 147 45.694 41.255 43.800 1.00 67.51 5776 C G LY D 147 45.694 41.255 45.701 1.00 62.13 5778 C G LY D 147 45.694 41.255 45.701 1.00 62.13 5778 C G LY D 147 45.694 41.255 45.701 1.00 62.13 5779 C G LY D 147 45.694 41.255 45.701 1.00 62.13 5778 C G LY D 147 45.694 41.255 45.701 1.00 62.13 5778 C G LY D 149 42.284 41.399 44.257 1.00 62.13 5778 C G LY D 149 42.894 41.399 41.500 1.00 62.13 5778 C G LY D 149 42.894 41.399 41.500 57.99 5780 C G LY R D 149 42.894 41.399 41.500 57.99 5780 C G LY R D 149 42.290 42.290		5750	N	GLU D						
7752 CB GLU D 144 41.492 39.011 55.003 1.00 215.80 7753 CG GLU D 144 41.840 39.428 55.363 1.00 215.80 7755 OE1 GLU D 144 40.992 39.001 57.475 1.00 215.80 7755 OE1 GLU D 144 41.555 39.596 56.416 1.00 215.80 7756 OE2 GLU D 144 41.555 39.596 56.416 1.00 215.80 7757 C GLU D 144 42.288 39.478 52.074 1.00 87.28 7758 O GLU D 144 42.288 39.478 52.074 1.00 87.28 7758 CA ASP D 145 41.533 42.083 51.491 1.00 67.03 7761 CB ASP D 145 39.484 43.320 52.163 1.00 129.44 7761 CB ASP D 145 39.484 43.320 52.163 1.00 129.44 7762 CG ASP D 145 39.684 43.320 52.163 1.00 129.44 7763 TF64 OD2 ASP D 145 39.168 43.899 53.229 1.00 129.44 7768 CA ASP D 145 44.8284 42.396 53.229 1.00 67.03 7769 CG ASP D 145 44.8284 42.396 53.229 1.00 129.44 7768 CG ASP D 145 44.8284 42.396 53.229 1.00 129.44 7768 CG ASP D 145 39.168 43.899 53.229 1.00 129.44 7768 CG ASP D 145 44.8284 42.396 53.229 1.00 129.44 7776 TF65 C ASP D 145 44.8284 42.396 53.229 1.00 129.44 7776 TF66 C ASP D 145 44.838 43.899 53.229 1.00 129.44 7776 TF66 C ASP D 145 44.838 43.899 53.229 1.00 129.44 7776 TF67 N SER D 146 43.802 42.121 51.177 1.00 89.85 7776 CA SER D 146 43.806 42.277 51.00 10.0 212.33 7777 C G SER D 146 44.810 39.333 49.895 1.00 18.885 7777 C G SER D 146 44.810 39.333 49.896 1.00 18.885 7778 C GLY D 147 45.696 41.256 48.213 1.00 67.51 7777 C G SER D 146 44.810 39.393 49.896 1.00 67.51 7777 C G GLY D 147 46.000 40.893 43.890 1.00 89.85 7770 C G SER D 146 44.810 39.393 49.896 1.00 67.51 7777 C G GLY D 147 46.000 40.893 43.890 1.00 65.25 7780 CG THR D 148 47.863 38.729 43.890 1.00 67.51 7777 C G GLY D 147 46.000 40.893 43.890 1.00 65.26 7780 CG THR D 148 47.963 39.898 44.895 1.00 67.51 7778 C G GLY D 147 46.000 40.893 45.865 1.00 67.51 7778 C G GLY D 147 46.000 40.893 45.865 1.00 67.51 7779 C G GLY D 147 46.000 40.893 43.890 1.00 62.13 45 5779 C G G THR D 148 47.963 39.898 44.895 1.00 62.13 7780 C G THR D 148 44.909 42.894 41.399 41.507 1.00 62.50 7780 C G THR D 149 42.899 44.102 41.500 40.000 1.00 42.86 7780 C TH7 D 149 40.000 40.899					144	42.603	39.874			
20 5754 CD GLU D 144 40.992 39.001 57.475 1.00 215.80 57.55 CD GLU D 144 40.992 39.001 57.475 1.00 215.80 57.56 CD GLU D 144 41.555 39.596 57.409 1.00 215.80 57.56 CD GLU D 144 41.555 39.596 58.416 1.00 215.80 57.55 CD GLU D 144 42.288 39.478 52.074 1.00 87.28 57.58 CD GLU D 144 42.288 39.478 52.074 1.00 87.28 57.58 CD GLU D 144 42.288 39.478 52.074 1.00 87.28 57.58 CD GLU D 144 42.288 39.478 52.074 1.00 87.28 57.58 CD GLU D 144 42.288 39.478 52.074 1.00 87.28 57.58 CD GLU D 145 42.288 39.478 52.074 1.00 87.28 57.58 CD GLU D 145 40.847 43.441 51.634 1.00 67.03 57.61 CB ASP D 145 40.847 43.441 51.634 1.00 129.44 57.62 CG ASP D 145 39.488 43.320 52.163 1.00 129.44 57.62 CG ASP D 145 39.488 43.320 52.163 1.00 129.44 57.62 CG ASP D 145 42.751 42.217 50.587 1.00 67.03 57.66 CD ASP D 145 42.751 42.217 50.587 1.00 67.03 57.66 CD ASP D 145 42.751 42.217 50.587 1.00 67.03 57.66 CD ASP D 145 42.751 42.217 50.587 1.00 67.03 57.67 N SER D 146 43.982 42.121 51.171 1.00 89.85 57.67 N SER D 146 43.982 42.121 51.171 1.00 89.85 57.69 CB SER D 146 48.366 42.277 51.300 1.00 120.33 57.71 CC SER D 146 48.317 43.408 52.152 1.00 212.33 57.71 C SER D 146 45.185 41.00 42.235 50.383 1.00 89.85 57.73 N GLY D 147 45.694 41.255 45.724 1.00 67.51 57.75 C GLY D 147 45.694 41.255 45.724 1.00 67.51 57.75 C GLY D 147 45.694 41.255 45.724 1.00 67.51 57.75 C GLY D 147 45.698 41.255 45.724 1.00 67.51 57.76 C GLY D 147 46.475 41.255 45.724 1.00 67.51 57.76 C GLY D 147 46.475 41.255 45.724 1.00 67.51 57.76 C GLY D 147 46.475 41.255 45.724 1.00 67.51 57.76 C GLY D 147 46.475 41.255 45.724 1.00 67.51 57.76 C GLY D 147 45.694 41.256 44.259 1.00 67.51 57.76 C GLY D 147 45.694 41.255 45.724 1.00 67.51 57.76 C GLY D 147 46.475 41.255 45.724 1.00 67.51 57.76 C GLY D 147 46.475 41.255 45.724 1.00 67.51 57.76 C GLY D 147 46.475 41.255 45.724 1.00 67.51 57.76 C GLY D 147 46.475 41.255 45.724 1.00 67.51 57.76 C GLY D 149 42.866 42.210 42.239 1.00 67.51 57.76 C GLY D 149 42.866 42.210 42.889 1.00 62.52 57.83 O GLY D 149 42.866 42.210 42.889 1.00 62.52 57.83 O G										
5755 OE1 GLU D 144 39.756 38.856 57.409 1.00 215.80 5756 OE2 GLU D 144 41.555 39.596 58.416 1.00 215.80 5757 C GLU D 144 42.245 40.287 52.992 1.00 87.28 5758 O GLU D 144 42.245 40.287 52.992 1.00 87.28 5758 O GLU D 144 42.288 39.478 52.074 1.00 87.28 5750 CA ASP D 145 41.593 42.083 51.491 1.00 67.03 5761 CB ASP D 145 40.847 43.200 52.163 1.00 129.44 5762 CG ASP D 145 39.448 43.320 52.163 1.00 129.44 5762 CG ASP D 145 39.448 43.320 52.163 1.00 129.44 5762 CG ASP D 145 39.448 43.320 52.163 1.00 129.44 5766 C ASP D 145 39.158 43.899 53.228 1.00 129.44 5766 C ASP D 145 39.158 43.899 53.228 1.00 129.44 5766 C ASP D 145 39.158 43.899 53.228 1.00 129.44 5766 C ASP D 145 39.158 43.899 53.228 1.00 129.44 5766 C ASP D 145 39.158 43.899 53.228 1.00 129.44 5766 C ASP D 145 39.158 43.899 53.228 1.00 129.44 5766 C ASP D 145 42.634 42.217 50.587 1.00 67.03 5766 O ASP D 145 42.634 42.217 50.587 1.00 67.03 5766 C ASP D 146 43.932 42.751 42.217 50.587 1.00 67.03 5766 C ASP D 146 43.932 42.751 42.217 50.587 1.00 67.03 5766 C ASP D 146 43.932 42.751 42.217 50.587 1.00 67.03 5768 CA SER D 146 45.165 42.235 50.883 1.00 89.85 5770 CG SER D 146 45.165 44.810 39.933 49.836 1.00 89.85 5771 C SER D 146 45.165 41.034 49.452 1.00 89.85 5771 C SER D 146 45.165 41.034 49.452 1.00 89.85 5771 C SER D 146 45.165 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 45.185 41.034 49.452 1.00 67.51 5777 C SER D 146 44.810 39.933 45.886 1.00 67.51 5777 C SER D 147 44.8000 40.893 45.865 1.00 67.51 5777 C SER D 147 44.8000 40.893 45	20									
5756	20									
5757 C GLU D 144 42.245 40.287 52.982 1.00 87.28 5758 O GLU D 144 42.245 40.287 52.982 1.00 87.28 5759 N ASP D 145 41.593 39.478 52.074 1.00 87.28 5760 CA ASP D 145 41.593 42.083 51.491 1.00 67.03 5761 CB ASP D 145 39.448 43.320 52.163 1.00 129.44 5762 CG ASP D 145 39.448 43.320 52.163 1.00 129.44 5763 OD1 ASP D 145 39.488 43.320 52.163 1.00 129.44 5766 C ASP D 145 39.158 43.999 53.228 1.00 129.44 5766 C ASP D 145 39.158 43.999 53.228 1.00 67.03 5766 O ASP D 145 39.158 43.999 53.228 1.00 67.03 5767 N SER D 146 42.634 42.396 49.365 1.00 67.03 5768 CA SER D 146 45.140 42.235 50.383 1.00 89.85 5768 CA SER D 146 45.140 42.235 50.383 1.00 89.85 5770 OG SER D 146 45.366 42.277 51.300 1.00 212.33 5771 C SER D 146 45.366 42.277 51.300 1.00 212.33 5772 O SER D 146 45.160 42.39 40.5773 N GLY D 147 45.604 41.256 48.213 1.00 67.51 5775 C GLY D 147 45.604 41.256 48.213 1.00 67.51 5776 C GLY D 147 45.604 41.256 48.213 1.00 67.51 5777 C GLY D 147 45.604 41.256 48.213 1.00 67.51 5776 C GLY D 147 45.604 41.256 48.213 1.00 67.51 5777 C GLY D 147 45.604 41.256 48.213 1.00 67.51 5778 CA THR D 148 45.975 40.327 43.454 1.00 67.51 5778 CA THR D 148 45.975 40.327 43.454 1.00 67.51 5778 CA THR D 148 47.073 39.493 42.270 1.00 62.13 5780 CG1 THR D 148 47.803 39.549 42.270 1.00 62.13 5780 CG1 THR D 148 47.803 39.549 42.270 1.00 62.13 5780 CG2 THR D 148 44.805 40.210 42.689 1.00 62.13 5780 CG2 THR D 148 44.806 40.210 42.689 1.00 62.13 5780 CG2 THR D 148 44.806 40.210 42.689 1.00 62.13 5780 CG2 THR D 149 42.894 41.399 42.250 1.00 42.86 5780 CG2 THR D 149 42.894 41.494 41.399 42.250 1.00 42.86 5780 CG2 THR D 149 42.698 42.693 39.596 1.00 42.86 5780 CG2 THR D 149 42.693 42.693 39.596 1.00 42.86 5780 CG1 THR D 149 42.693 42.693 42.693 1.00 62.13 5780 CG1 THR D 148 43.093 42.693 43.690 1.00 62.13 5780 CG2 THR D 149 42.693 42.693 42.693 1.00 42.86 5780 CG2 THR D 149 42.693 42.693 42.693 1.00 62.13 5780 CG1 THR D 149 42.693 42.693 42.693 1.00 62.693 5780 CG1 THR D 149 42.693 42.693 42.693 39.800 1.00 57.99 5780 CG1 THR D 149 42.693 42.693 42.693										
25 5759 N ASP D 145 41.539 41.556 52.074 1.00 67.03 5760 CA ASP D 145 41.593 42.083 51.491 1.00 67.03 5761 CB ASP D 145 40.847 43.441 51.634 1.00 129.44 5762 CG ASP D 145 39.448 43.220 52.163 1.00 129.44 5762 CG ASP D 145 39.448 43.220 52.163 1.00 129.44 5763 0D1 ASP D 145 39.488 43.220 52.163 1.00 129.44 5763 0D1 ASP D 145 39.586 42.636 51.510 1.00 67.03 5764 OD2 ASP D 145 39.158 43.899 53.228 1.00 129.44 5765 C ASP D 145 42.751 42.217 50.587 1.00 67.03 5766 O ASP D 145 42.751 42.217 50.587 1.00 67.03 5766 O ASP D 145 42.751 42.217 50.587 1.00 67.03 5766 CA SER D 146 43.932 42.121 51.177 1.00 89.85 5769 CB SER D 146 45.140 42.235 50.383 1.00 10.0 212.33 5771 C SER D 146 45.140 42.237 51.300 1.00 212.33 5771 C SER D 146 45.185 41.034 49.455 1.00 212.33 5771 C SER D 146 45.185 41.034 49.455 1.00 89.85 5772 O SER D 146 44.810 39.933 49.836 1.00 67.51 5772 O SER D 146 44.810 39.933 49.836 1.00 67.51 5775 C GLy D 147 45.694 41.256 48.213 1.00 67.51 5776 C GLY D 147 45.694 41.256 48.213 1.00 67.51 5776 C GLY D 147 45.694 41.256 48.213 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 45.865 1.00 67.51 5776 C GLY D 147 48.000 40.693 37.549 40.300 1.00 42.86 57										
25 5759 N	~ ~	5758	0							
5762 CG ASP D 145 39.448 43.320 52.153 1.00 129.44 5763 OD1 ASP D 145 39.448 43.320 52.153 1.00 129.44 5763 OD1 ASP D 145 38.636 42.636 51.510 1.00 129.44 5766 C ASP D 145 38.636 42.636 51.510 1.00 129.44 5766 C ASP D 145 42.751 42.217 50.587 1.00 67.03 5766 O ASP D 145 42.751 42.217 50.587 1.00 67.03 5766 O ASP D 145 42.751 42.217 50.587 1.00 67.03 5766 O ASP D 145 42.634 42.396 49.365 1.00 67.03 5766 O ASP D 146 43.932 42.121 51.177 1.00 89.85 5768 CB SER D 146 43.932 42.121 51.177 1.00 89.85 5768 CB SER D 146 45.140 42.235 50.383 1.00 89.85 5770 OG SER D 146 48.317 43.408 52.152 1.00 212.33 5771 C SER D 146 48.317 43.408 52.152 1.00 212.33 5771 C SER D 146 44.810 39.933 49.856 1.00 89.85 5772 O SER D 146 44.810 39.933 49.856 1.00 89.85 5773 N GLY D 147 45.698 40.184 47.254 1.00 67.51 5775 C GLY D 147 45.698 40.184 47.254 1.00 67.51 5775 C GLY D 147 48.400 40.893 45.865 1.00 67.51 5776 O GLY D 147 48.400 40.893 45.865 1.00 67.51 5777 N THR D 148 45.740 39.888 44.855 1.00 67.51 5777 CB THR D 148 47.073 39.493 42.277 1.00 62.13 5779 CB THR D 148 47.073 39.493 42.277 1.00 62.13 5779 CB THR D 148 47.073 39.493 42.277 1.00 62.13 5780 OG1 THR D 148 47.073 39.493 42.277 1.00 62.13 5780 OG1 THR D 148 47.863 38.564 41.871 1.00 67.51 5780 OG1 THR D 148 47.073 39.493 42.277 1.00 62.13 5780 OG1 THR D 148 47.865 40.210 42.889 1.00 62.13 5780 CB THR D 148 44.865 40.210 42.889 1.00 62.13 5780 CB THR D 148 44.865 40.210 42.889 1.00 62.13 5780 CB THR D 149 42.894 41.399 41.547 1.00 62.13 5780 CB THR D 149 42.894 41.399 41.547 1.00 62.13 5780 CB THR D 149 42.894 41.399 41.547 1.00 62.13 5780 CB THR D 149 42.894 41.399 41.547 1.00 62.13 5780 CB THR D 149 42.894 41.399 41.547 1.00 62.13 5780 CB THR D 149 42.894 41.399 42.200 1.00 42.86 5781 CG2 THR D 149 42.894 41.399 42.200 1.00 42.86 5781 CG2 THR D 149 42.894 41.399 42.200 1.00 42.86 5781 CG2 THR D 149 42.894 41.399 42.200 1.00 42.86 5789 CB TYR D 149 40.089 42.570 40.237 40.940 1.00 42.86 5789 CB TYR D 149 40.089 42.570 40.237 40.940 1.00 42.86 5789 CB TYR D 149 40.089 42.570	25				45	41.898				
5762										
30 5783 OD1 ASP D 145 38.836 42.836 51.510 1.00 129.44 5785 C ASP D 145 38.836 42.836 51.510 1.00 129.44 5786 C ASP D 145 42.751 42.217 50.587 1.00 67.03 5786 O ASP D 145 42.751 42.217 50.587 1.00 67.03 5786 O ASP D 145 42.634 42.396 49.365 1.00 67.03 5787 N SER D 146 43.932 42.121 51.177 1.00 89.85 5788 CA SER D 146 45.140 42.235 50.383 1.00 89.85 5789 CB SER D 146 45.140 42.235 50.383 1.00 89.85 5770 OG SER D 146 45.140 42.235 50.383 1.00 89.85 5770 OG SER D 146 46.317 43.408 52.152 1.00 212.33 5771 C SER D 146 44.810 39.933 49.836 1.00 89.85 5772 O SER D 146 44.810 39.933 49.836 1.00 89.85 5773 N GLY D 147 45.604 41.256 48.213 1.00 67.51 5776 C GLY D 147 45.604 41.256 48.213 1.00 67.51 5775 C GLY D 147 45.604 41.256 48.213 1.00 67.51 5776 O GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 N THR D 148 45.754 49.836 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 67.51 5776 C GLY D 147 46.000 40.683 45.865 1.00 62.13 5786 CA THR D 148 45.740 39.888 44.835 1.00 62.13 5786 CA THR D 148 47.863 38.729 43.800 1.00 62.13 5786 CA THR D 148 44.864 33.80.564 41.871 1.00 62.13 5780 CG THR D 148 44.864 33.80.564 41.871 1.00 62.13 5785 CA THR D 148 44.866 40.210 42.889 1.00 42.86 5783 CA THR D 149 42.079 42.524 43.800 1.00 42.86 5783 CA THR D 149 42.079 42.524 43.800 1.00 42.86 5783 CA THR D 149 42.079 42.524 43.800 1.00 42.86 5783 CA THR D 149 42.079 42.524 47.568 1.00 42.86 5783 CA THR D 149 42.079 42.524 47.568 1.00 42.86 5783 CA THR D 149 42.089 42.662 44.522 1.00 42.86 5783 CA THR D 149 42.089 42.662 44.522 1.00 42.86 5783 CA THR D 149 42.089 42.662 44.522 1.00 42.86 5783 CA THR D										
30 5764 OD2 ASP D 145 39.158 43.899 53.228 1.00 129.44 5766 C ASP D 145 42.751 42.217 50.587 1.00 67.03 5766 O ASP D 145 42.634 42.396 49.365 1.00 67.03 5768 CA SER D 146 43.932 42.121 51.177 1.00 89.85 5768 CA SER D 146 45.140 42.235 50.383 1.00 89.85 5770 OG SER D 146 45.185 41.034 89.452 1.00 212.33 5771 C SER D 146 45.185 41.034 89.452 1.00 89.85 5772 O SER D 146 45.185 41.034 89.452 1.00 89.85 5773 N GLY D 147 45.694 41.256 48.213 1.00 67.51 5776 <td></td>										
5765 C ASP D 145 42.751 42.217 50.587 1.00 67.03 5766 O ASP D 145 42.634 42.396 49.365 1.00 67.03 5767 N SER D 146 43.932 42.121 51.177 1.00 89.85 5768 CA SER D 146 45.140 42.235 50.383 1.00 89.85 5770 OG SER D 146 46.317 43.408 52.152 1.00 212.33 5771 C SER D 146 46.317 43.408 52.152 1.00 89.85 5772 O SER D 146 44.810 39.933 49.836 1.00 89.85 5773 N GLY D 147 45.698 40.164 47.254 1.00 67.51 5774 CA GLY D 147 46.600 40.633 45.865 1.00 67.51 5775 C	30									
5766 O ASP D 145 42,634 42,396 49,365 1.00 67,03 5768 CA SER D 146 43,332 42,121 51,177 1.00 89,85 5769 CA SER D 146 45,140 42,235 50,383 1.00 89,85 5770 OG SER D 146 48,366 42,277 51,300 1.00 212,33 5771 C SER D 146 45,185 41,034 49,452 1.00 89,85 5772 O SER D 146 45,185 41,034 49,452 1.00 89,85 5773 N GLY D 147 45,694 41,256 48,213 1.00 67,51 5775 C GLY D 147 46,000 40,683 45,865 1.00 67,51 5776 O GLY D 147 46,075										
5768 CA SER D 146 43,932 42,121 51,177 1.00 89,85 5768 CA SER D 146 45,140 42,235 50,383 1.00 89,85 5768 CB SER D 146 45,140 42,235 50,383 1.00 89,85 5770 CG SER D 146 46,317 43,408 52,152 1.00 212,33 5770 C SER D 146 46,317 43,408 52,152 1.00 212,33 5771 C SER D 146 44,810 39,933 49,836 1.00 89,85 5772 C SER D 146 44,810 39,933 49,836 1.00 89,85 5773 N GLY D 147 45,604 41,256 48,213 1.00 67,51 5775 C GLY D 147 46,000 40,693 45,665 1.00 67,51 5776 O GLY D 147 46,000 40,693 45,665 1.00 67,51 5777 N THR D 148 45,740 39,885 45,724 1.00 67,51 5777 N THR D 148 45,740 39,885 44,835 1.00 62,13 5778 CA THR D 148 45,740 39,884 44,835 1.00 62,13 5778 CB THR D 148 45,740 39,884 44,835 1.00 62,13 5778 CB THR D 148 45,740 39,884 44,835 1.00 62,13 5778 CG THR D 148 47,073 39,893 42,770 1.00 85,26 5780 OG1 THR D 148 46,833 38,564 41,871 1.00 85,26 5781 CG2 THR D 148 47,863 38,729 43,800 1.00 85,26 5782 C THR D 148 44,665 40,210 42,689 1.00 62,13 5783 O THR D 148 44,166 41,339 42,220 1.00 62,13 5783 O THR D 149 44,164 41,339 42,220 1.00 62,13 5786 CB TYR D 149 44,164 41,349 41,547 1.00 62,13 5786 CB TYR D 149 42,689 42,662 44,522 1.00 42,86 5790 CD2 TYR D 149 42,639 42,702 45,880 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 149 40,008 42,412 45,511 1.00 42,86 5790 CD2 TYR D 150 41,921 41,262 39,340 1.00 57,99 5790 CD2 TYR D 150 41,921 41,262 39,		5766	0							
35 5769 CB SER D 146 46.366 42.277 51.300 1.00 212.33 5770 OG SER D 146 46.317 43.408 52.152 1.00 212.33 5771 C SER D 146 45.185 41.034 49.452 1.00 89.85 5772 O SER D 146 44.810 39.933 49.836 1.00 89.85 5773 N GLY D 147 45.604 41.256 48.213 1.00 67.51 5775 C GLY D 147 46.600 40.693 45.865 1.00 67.51 5776 O GLY D 147 46.475 41.825 45.724 1.00 67.51 5777 N THR D 148 45.975 40.327 43.454 1.00 62.13 45 5779 CB THR D 148 45.975 40.327 43.454 1.00 62.13						43.932	42.121			
5770 OG SER D 146 46.317 43.408 \$2.152 1.00 212.33 5771 C SER D 146 45.185 41.034 49.452 1.00 89.85 5772 O SER D 146 44.810 39.933 49.836 1.00 689.85 5773 N GLY D 147 45.604 41.256 48.213 1.00 67.51 5774 CA GLY D 147 45.698 40.164 47.254 1.00 67.51 5775 C GLY D 147 46.000 40.693 45.865 1.00 67.51 5776 O GLY D 147 46.475 41.825 45.724 1.00 67.51 5776 TRIR D 148 45.975 40.327 43.454 1.00 62.13 45 5778 CB THR D 148 47.073 39.493 42.770 1.00 85.26 5781	25									89.85
5771 C SER D 146 45.185 41.034 49.452 1.00 89.85 5772 O SER D 146 44.810 39.933 49.836 1.00 89.85 5773 N GLY D 147 45.694 41.256 48.213 1.00 67.51 5775 C GLY D 147 45.698 40.164 47.254 1.00 67.51 5776 O GLY D 147 46.000 40.693 45.865 1.00 67.51 5777 N THR D 148 45.740 39.888 44.835 1.00 67.51 5777 N THR D 148 45.740 39.888 44.835 1.00 62.13 5778 CA THR D 148 45.975 40.327 43.454 1.00 62.13 5778 CA THR D 148 45.975 40.327 43.454 1.00 62.13 5778 CA THR D 148 46.83 38.564 41.871 1.00 62.13 5780 OG1 THR D 148 46.83 38.564 41.871 1.00 85.26 5781 CG2 THR D 148 47.863 38.729 43.800 1.00 85.26 5782 C THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.106 39.134 42.527 1.00 62.13 5784 N TYR D 149 44.164 41.339 42.230 1.00 62.13 5785 CA TYR D 149 42.894 41.349 41.547 1.00 62.15 5787 CG TYR D 149 42.689 42.662 44.522 1.00 42.86 5780 CD1 TYR D 149 42.689 42.662 44.522 1.00 42.86 5790 CD2 TYR D 149 42.689 42.662 44.522 1.00 42.86 5790 CD2 TYR D 149 40.038 42.702 45.880 1.00 42.86 5790 CD2 TYR D 149 40.038 42.702 45.880 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5790 CD2 TYR D 149 40.003 42.609 42.609 42.600 40.006 1.00 42.86 5790 CD2 TYR D 150 41.799 41.429 37.892 1.00 57.99 5790 CD TYR D 150 42.804 37.342 36.010 1.00 88.00 5800 CD1 TYR D 150 4	<i>JJ</i>									
5772 O SER D 146 44.810 39.933 49.836 1.00 89.85 5773 N GLY D 147 45.604 41.256 48.213 1.00 67.51 5774 CA GLY D 147 45.698 40.164 47.254 1.00 67.51 5775 C GLY D 147 46.000 40.693 45.865 1.00 67.51 5776 O GLY D 147 46.475 41.825 45.724 1.00 67.51 5777 N THR D 148 45.740 39.888 44.835 1.00 62.13 5778 CA THR D 148 45.795 40.327 43.454 1.00 62.13 5778 CB THR D 148 47.073 39.493 42.770 1.00 85.26 5780 OG1 THR D 148 47.073 39.493 42.770 1.00 85.26 5781 CG2 THR D 148 47.863 38.729 43.800 1.00 85.26 5782 C THR D 148 44.665 40.210 42.689 1.00 62.13 5788 O THR D 148 44.665 40.210 42.689 1.00 62.13 5785 CA TYR D 149 44.164 41.339 42.230 1.00 42.52 5786 CB TYR D 149 44.164 41.339 42.230 1.00 42.52 5786 CB TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.498 43.543 1.00 42.86 5787 CG TYR D 149 42.072 42.498 43.543 1.00 42.86 5789 CD1 TYR D 149 42.689 42.602 44.522 1.00 42.86 5780 CD2 TYR D 149 42.039 42.702 45.880 1.00 42.86 5780 CD2 TYR D 149 40.038 42.470 45.883 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5780 CD2 TYR D 149 40.038 42.412 45.251 1.00 57.99 5796 CB TYR D 149 40.038 42.412 45.251 1.00 57.99 5798 CB TYR D 150 41.921 41.847 39.556 1.00 57.99 5798 CB TYR D 150 41.921 41.242 39.356 1.00 57.99 5798 CB TYR D 150 42.875 40.420 37.081 1.00 57.99 5798 CB TYR D 150 42.863 37.342 38.601 1.00 58.00 5800 CD1 TYR D 150 42.863 37.342 38.601 1.00 88.00 5800 CD1 TYR D 150 42.863 37.342 38.601 1.00 88.00 5800 CD1 TYR D 150 42.863 37.342 38.606 37.513 1.00 88.00 5802 CD2 TYR D 150 42.422 38.626 37.513 1.00 88.00										
40 5773 N GLY D 147 45.694 41.256 48.213 1.00 67.51 5774 CA GLY D 147 45.698 40.164 47.254 1.00 67.51 5775 C GLY D 147 46.000 40.893 45.865 1.00 67.51 5776 O GLY D 147 46.475 41.825 45.724 1.00 67.51 5776 N THR D 148 45.740 39.888 44.835 1.00 62.13 5778 CA THR D 148 45.975 40.327 43.454 1.00 62.13 5778 CA THR D 148 45.975 40.327 43.454 1.00 62.13 5778 CB THR D 148 47.073 39.493 42.770 1.00 85.26 5780 OG1 THR D 148 47.073 39.493 42.770 1.00 85.26 5781 CG2 THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.106 39.134 42.527 1.00 62.13 5785 CA TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.55 5787 CG TYR D 149 42.072 42.518 43.543 1.00 42.86 5782 CD TYR D 149 42.072 42.518 43.543 1.00 42.86 5782 CD TYR D 149 42.039 42.662 44.522 1.00 42.86 5782 CD TYR D 149 42.039 42.662 44.522 1.00 42.86 5781 CE2 TYR D 149 42.039 42.662 44.522 1.00 42.86 5781 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5781 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5782 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 149 40.038 42.412 45.251 1.00 42.86 5783 CD TYR D 150 42.86 37.342 30.600 1.00 5										
40 5774 CA GLY D 147 45.698 40.164 47.254 1.00 67.51 5775 C GLY D 147 46.000 40.693 45.865 1.00 67.51 5776 O GLY D 147 46.000 40.693 45.865 1.00 67.51 5776 O GLY D 147 46.475 41.825 45.724 1.00 67.51 5777 N THR D 148 45.740 39.888 44.835 1.00 62.13 5778 CA THR D 148 45.975 40.327 43.454 1.00 62.13 5778 CB THR D 148 45.975 40.327 43.454 1.00 62.13 5779 CB THR D 148 47.073 39.493 42.770 1.00 85.26 5781 CG2 THR D 148 46.483 38.564 41.871 1.00 85.26 5781 CG2 THR D 148 47.863 38.729 43.800 1.00 85.26 5782 C THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.104 39.134 42.527 1.00 62.13 5785 CA TYR D 149 44.164 41.339 42.230 1.00 42.52 5785 CA TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 42.689 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 42.689 42.662 44.522 1.00 42.86 5789 CD1 TYR D 149 42.639 42.702 45.880 1.00 42.86 5789 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5789 CD2 TYR D 149 40.003 42.702 45.880 1.00 42.86 5789 CD2 TYR D 149 40.003 42.404 42.373 43.936 1.00 42.86 5789 CD2 TYR D 149 40.003 42.412 45.251 1.00 42.86 5789 CD2 TYR D 149 40.003 42.412 45.251 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 45.800 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 149 40.998 42.570 46.237 1.00 42.86 5789 CD2 TYR D 150 42.860 37.342 39.340 1.00 57.99 5799 CA TYR D 150 42.860 37.342 39.3661 36.156 1.00 88.00 5800 CD1 TYR D 150 42.860 37.342 38.661 36.156 1.00 88.0										
5775 C GLY D 147 46.000 40.693 45.865 1.00 67.51 5776 O GLY D 147 46.475 41.825 45.724 1.00 67.51 5777 N THR D 148 45.740 39.888 44.835 1.00 62.13 5778 CA THR D 148 45.975 40.327 43.454 1.00 62.13 45 5779 CB THR D 148 47.073 39.493 42.770 1.00 62.52 5780 OG1 THR D 148 47.073 39.493 42.770 1.00 65.26 5781 CG2 THR D 148 47.883 38.729 43.800 1.00 85.26 5782 C THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.106 39.134 42.527 1.00 62.13 5784 N TYR D 149 44.164 41.339 42.220 1.00 62.13 5785 CA TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.55 5787 CG TYR D 149 42.072 42.518 43.543 1.00 42.86 5780 CD1 TYR D 149 42.689 42.662 44.522 1.00 42.86 5780 CD2 TYR D 149 42.689 42.662 44.522 1.00 42.86 5790 CD2 TYR D 149 40.038 42.402 45.880 1.00 42.86 5790 CD2 TYR D 149 40.038 42.570 45.281 1.00 42.86 5790 CD2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5791 CE2 TYR D 149 40.038 42.570 46.237 1.00 42.86 5792 CZ TYR D 149 40.038 42.570 45.237 1.00 42.86 5793 OH TYR D 149 40.038 42.570 46.237 1.00 42.86 5794 C TYR D 149 40.038 42.570 46.237 1.00 42.86 5795 CD TYR D 149 40.038 42.570 46.237 1.00 42.86 5790 CD2 TYR D 149 40.038 42.570 46.237 1.00 42.86 5791 CE2 TYR D 149 40.038 42.570 46.237 1.00 42.86 5792 CZ TYR D 149 40.038 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.038 42.570 46.237 1.00 42.86 5795 CA TYR D 149 40.038 42.570 46.237 1.00 42.86 5796 N TYR D 149 40.038 42.570 46.237 1.00 57.99 5797 CA TYR D 149 40.038 42.570 46.237 1.00 57.99 5798 CB TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD1 TYR D 150 42.422 38.661 38.156 1.00 88.00 5800 CD1 TYR D 150 42.422 36.626 37.513 1.00 88.00	40				147					
5777 N THR D 148 45.740 39.888 44.835 1.00 62.13 5778 CA THR D 148 45.975 40.327 43.454 1.00 62.13 5779 CB THR D 148 45.975 40.327 43.454 1.00 62.13 5780 OG1 THR D 148 47.073 39.493 42.770 1.00 65.26 5781 CG2 THR D 148 46.83 38.564 41.871 1.00 65.26 5782 C THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.106 39.134 42.527 1.00 62.13 50 5784 N TYR D 149 44.164 41.339 42.230 1.00 42.52 5785 CA TYR D 149 44.164 41.339 42.230 1.00 42.52 5786 CB TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 42.689 42.662 44.522 1.00 42.86 5789 CD1 TYR D 149 42.689 42.662 44.522 1.00 42.86 5780 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5790 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.592 42.542 45.251 1.00 42.86 5793 OH TYR D 149 40.598 42.570 46.237 1.00 42.86 5794 C TYR D 149 40.592 42.542 47.568 1.00 42.86 5795 O TYR D 149 40.592 42.542 47.568 1.00 42.86 5796 N TYR D 149 40.592 42.542 47.568 1.00 42.86 5796 N TYR D 149 40.592 42.542 39.340 1.00 57.99 5797 CA TYR D 149 40.592 42.542 39.340 1.00 57.99 5798 CB TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5801 CE1 TYR D 150 42.2840 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5803 CE2 TYR D 150 42.422 36.626 37.513 1.00 88.00								45.865		
45 5778 CA THR D 148 45.975 40.327 43.454 1.00 62.13 5779 CB THR D 148 47.073 39.493 42.770 1.00 85.26 5780 OG1 THR D 148 46.483 38.564 41.871 1.00 85.26 5781 CG2 THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.106 39.134 42.527 1.00 62.13 5785 CA TYR D 149 44.106 39.134 42.527 1.00 62.13 5785 CA TYR D 149 42.072 42.518 42.079 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 42.339 42.662 44.522 1.00 42.86 5780 CD1 TYR D 149 42.339 42.702 45.880 1.00 42.86 5780 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5790 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5793 OH TYR D 149 40.998 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.998 42.570 46.237 1.00 42.86 5793 OH TYR D 149 43.028 41.506 40.046 1.00 42.56 5793 OH TYR D 149 43.028 41.506 40.046 1.00 42.56 5793 OH TYR D 149 43.028 41.506 40.046 1.00 42.56 5793 OH TYR D 149 43.028 41.506 40.046 1.00 42.56 5793 OH TYR D 149 43.028 41.506 40.046 1.00 42.56 5794 C TYR D 149 43.028 41.506 40.046 1.00 57.99 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.921 41.262 39.340 1.00 57.99 5798 CB TYR D 150 41.921 41.262 39.340 1.00 57.99 5798 CB TYR D 150 41.921 41.262 39.340 1.00 57.99 5798 CB TYR D 150 41.921 41.262 39.340 1.00 57.99 5799 CG TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.675 40.420 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.84										
45 5779 CB THR D 148 47.073 39.493 42.770 1.00 85.26 5780 OG1 THR D 148 46.483 38.564 41.871 1.00 85.26 5781 CG2 THR D 148 47.863 38.729 43.800 1.00 85.26 5782 C THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.106 39.134 42.527 1.00 62.13 5783 CA TYR D 149 44.164 41.339 42.230 1.00 42.52 5785 CA TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 42.689 42.662 44.522 1.00 42.86 5787 CG TYR D 149 42.689 42.662 44.522 1.00 42.86 5787 CG TYR D 149 42.339 42.662 44.522 1.00 42.86 5780 CD1 TYR D 149 42.339 42.702 45.880 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5793 OH TYR D 149 40.038 42.412 45.251 1.00 42.86 5793 OH TYR D 149 40.038 42.412 45.251 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5794 C TYR D 149 40.592 42.542 47.568 1.00 42.86 5794 C TYR D 149 40.592 42.542 47.568 1.00 42.86 5794 C TYR D 149 40.592 42.542 39.340 1.00 57.99 5795 O TYR D 149 43.028 41.506 40.046 1.00 42.552 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.921 41.262 39.340 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00 5800 CD2 TYR D 150 42.422 36.6										
5780 OG1 THR D 148 46.483 33.564 41.871 1.00 85.26 5781 CG2 THR D 148 47.863 38.729 43.800 1.00 85.26 5782 C THR D 148 44.665 40.210 42.689 1.00 62.13 5783 O THR D 148 44.106 39.134 42.527 1.00 62.13 5784 N TYR D 149 44.164 41.339 42.230 1.00 42.52 5785 CA TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 41.722 42.498 43.543 1.00 42.86 5787 CG TYR D 149 42.689 42.662 44.522 1.00 42.86 5787 CG TYR D 149 42.339 42.702 45.880 1.00 42.86 5780 CD1 TYR D 149 42.339 42.702 45.880 1.00 42.86 5790 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5790 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5792 CZ TYR D 149 40.998 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5793 OH TYR D 150 41.921 41.262 39.340 1.00 57.99 5796 N TYR D 150 41.791 41.262 39.340 1.00 57.99 5798 CB TYR D 150 41.791 41.262 39.340 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.840 37.342 36.010 1.00 88.00 5800 CD1 TYR D 150 42.843 37.342 36.010 1.00 88.00 5800 CD1 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5800 CD2 TYR D 150 42.422 36.626 37.513 1.00 88.00	45									
5781	-									
5782			CG2	THR D						
50 5784 N TYR D 149 44.164 41.339 42.230 1.00 42.52 5785 CA TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 42.689 42.662 44.522 1.00 42.86 5783 CD1 TYR D 149 42.689 42.662 44.522 1.00 42.86 5793 CE1 TYR D 149 42.339 42.702 45.880 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5791 CE2 TYR D 149 40.038 42.570 46.237 1.00 42.86 5792 CZ TYR D 149 <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>42.689</td> <td>1.00</td> <td></td>								42.689	1.00	
5785 CA TYR D 149 42.894 41.349 41.547 1.00 42.52 5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 41.722 42.498 43.543 1.00 42.86 5783 CD1 TYR D 149 42.689 42.662 44.522 1.00 42.86 5789 CE1 TYR D 149 42.339 42.702 45.880 1.00 42.86 5790 CD2 TYR D 149 40.339 42.702 45.880 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5793 OH TYR D 149 40.998 42.570 46.237 1.00 42.86 5794 C TYR D 149 40.592 42.542 47.568 1.00 42.86 5795 C TYR D 149 40.592 42.542 47.568 1.00 42.86 5796 N TYR D 149 43.028 41.506 40.046 1.00 42.52 5796 N TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.921 41.262 39.340 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 42.840 37.948 37.649 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00	50									62 .13
5786 CB TYR D 149 42.072 42.518 42.079 1.00 42.86 5787 CG TYR D 149 41.722 42.498 43.543 1.00 42.86 5783 CD1 TYR D 149 42.689 42.662 44.522 1.00 42.86 5790 CD2 TYR D 149 42.339 42.702 45.880 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.998 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5794 C TYR D 149 40.592 42.542 47.568 1.00 42.86 5795 O TYR D 149 43.028 41.506 40.046 1.00 42.52 5796 N TYR D 149 44.102 41.847 39.556 1.00 57.99 5797 CA TYR D 150 41.921 41.262 39.340 1.00 57.99 5798 CB TYR D 150 41.799 41.429 37.892 1.00 57.99 5799 CG TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.675 40.420 37.108 1.00 88.00 5801 CE1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00	20									
5787 CG TYR D 149 41.722 42.498 43.543 1.00 42.86 5783 CD1 TYR D 149 42.689 42.662 44.522 1.00 42.86 5753 CE1 TYR D 149 42.339 42.702 45.880 1.00 42.86 5790 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.098 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5794 C TYR D 149 43.028 41.506 40.046 1.00 42.52 5795 O TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.921 41.262 39.340 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.892 1.00 57.99 5799 CG TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5801 CE1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00										
5783 CD1 TYR D 149 42.689 42.662 44.522 1.00 42.86 5780 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5790 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.998 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5794 C TYR D 149 40.592 42.542 47.568 1.00 42.86 5795 O TYR D 149 43.028 41.506 40.046 1.00 42.52 5796 N TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.921 41.262 39.340 1.00 57.99 5798 CB TYR D 150 41.789 41.429 37.892 1.00 57.99 5799 CG TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5801 CE1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00										
55 5769 CE1 TYR D 149 42.339 42.702 45.880 1.00 42.86 5790 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.998 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 60 5794 C TYR D 149 43.028 41.506 40.046 1.00 42.86 5795 O TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D										
5790 CD2 TYR D 149 40.404 42.373 43.936 1.00 42.86 5791 CE2 TYR D 149 40.038 42.412 45.251 1.00 42.86 5792 CZ TYR D 149 40.998 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5794 C TYR D 149 43.028 41.506 40.046 1.00 42.52 5795 O TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.789 41.429 37.892 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5801 CE1 TYR D 150 42.840 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00	55			TYR D						
5792 CZ TYR D 149 40.998 42.570 46.237 1.00 42.86 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 60 5794 C TYR D 149 43.028 41.506 40.046 1.00 42.52 5795 O TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.799 41.429 37.892 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5709 CG TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5801 CE1 TYR D 150 40.693 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00				TYR D				43.936		
60 5793 OH TYR D 149 40.592 42.542 47.568 1.00 42.86 5794 C TYR D 149 43.028 41.506 40.046 1.00 42.52 5795 O TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.799 41.429 37.892 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5799 CG TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 41.124 38.661 36.156 1.00 88.00 5801 CE1 TYR D 150										
60 5794 C TYR D 149 43.028 41.506 40.046 1.00 42.52 5795 O TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.799 41.429 37.892 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5799 CG TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 41.124 38.661 36.156 1.00 88.00 5801 CE1 TYR D 150 42.840 37.948 37.649 1.00 88.00 5802 CD2 TYR D 150				TYPE						
5795 O TYR D 149 44.102 41.847 39.556 1.00 42.52 5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.799 41.429 37.892 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 57.99 CG TYR D 150 42.197 38.986 36.975 1.00 88.00 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 41.124 38.661 36.156 1.00 88.00 5801 CE1 TYR D 150 40.683 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5803 CE2 TYR D 150 42.840 37.948 37.649 1.00 88.00	60			TYRD						
5796 N TYR D 150 41.921 41.262 39.340 1.00 57.99 5797 CA TYR D 150 41.799 41.429 37.892 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 57.99 CG TYR D 150 42.197 38.986 36.975 1.00 88.00 CD1 TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 41.124 38.661 36.156 1.00 88.00 5801 CE1 TYR D 150 40.683 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5803 CE2 TYR D 150 42.422 36.626 37.513 1.00 88.00										
5797 CA TYR D 150 41.799 41.429 37.892 1.00 57.99 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5799 CG TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 41.124 38.661 36.156 1.00 88.00 5801 CE1 TYR D 150 41.693 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5803 CE2 TYR D 150 42.422 36.626 37.513 1.00 88.00		5796	N	TYR D						
65 5798 CB TYR D 150 42.675 40.420 37.108 1.00 88.00 5799 CG TYR D 150 42.197 38.986 36.975 1.00 88.00 5800 CD1 TYR D 150 41.124 38.661 36.156 1.00 88.00 5801 CE1 TYR D 150 40.683 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5803 CE2 TYR D 150 42.422 36.626 37.513 1.00 88.00				TYR D						
5800 CD1 TYR D 150 41.124 38.661 36.156 1.00 88.00 5801 CE1 TYR D 150 40.693 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5803 CE2 TYR D 150 42.422 36.626 37.513 1.00 88.00	65								1.00	88.00
5801 CE1 TYR D 150 40.683 37.342 36.010 1.00 88.00 5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5803 CE2 TYR D 150 42.422 36.626 37.513 1.00 88.00	U)									
5802 CD2 TYR D 150 42.840 37.948 37.649 1.00 88.00 5803 CE2 TYR D 150 42.422 36.626 37.513 1.00 88.00										
70 5803 CE2 TYR D 150 42.422 36.626 37.513 1.00 88.00										
7(1) 5004 07 500 0			CE2							
	70	5804	CZ	TYR D	150					

	5805	ОН	TYR D	150	40.898	35.020	36.578	1.00	00.00
	5806	Č.	TYR D	150	40.293	41.260	37.623	1.00	88.00 57.99
	5807	0	TYR D	150	39.569	40.702	38.470	1.00	57.99
5	5808	N	CYS D	151	39.783	41.782	36.500	1.00	62.97
J	5809 5810	CA C	CYS D CYS D	151 151	38.365 38.136	41.650 41.175	36.193 34.780	1.00	62.97
	5811	ŏ	CYS D	151	39.009	41.75	33.931	1.00 1.00	62.97 62.97
	5812	СВ	CYS D	151	37.636	42.966	36.413	1.00	102.16
	5813	SG	CYS D	151	38.287	44.417	35.527	1.00	102.16
10	5814	N	THR D	152	36.975	40.566	34.538	1.00	73.20
	5815 5816	CA CB	THR D	152	36.613	40.055	33.215	1.00	73.20
	5817	OG1	THR D	152 152	36.437 35.288	38.527 38.183	33.230 34.017	1.00 1.00	136.00 136.00
	5818	CG2	THR D	152	37.664	37.855	33.814	1.00	136.00
15	5819	С	THR D	152	35.286	40.688	32.830	1.00	73.20
	5820	0	THR D	152	34.434	40.945	33.698	1.00	73.20
	5821 5822	N CA	GLY D GLY D	153 153	35.105 33.863	40.950 41.572	31.538 31.099	1.00 1.00	64.84 64.84
	5823	č	GLY D	153	33.682	41.463	29.609	1.00	64.84
20	5824	0	GLY D	153	34.636	41.184	28.899	1.00	64.84
	5825	N	LYS D	154	32.462	41.680	29.133	1.00	72.61
	5826 5827	CA CB	LYS D LYS D	154 154	32.180 30.881	41.576	27.706	1.00	72.61
	5828	CG	LYS D	154	30.546	40.800 40.515	27.484 26.030	1.00 1.00	205.73 205.73
25	5829	CD	LYS D	154	29.274	39.697	25.956	1.00	205.73
	5830	CE	LYS D	154	C2 825	39.439	24.533	1.00	205.73
	5831	NZ	LYS D	154	27.516	38.730	24.533	1.00	205.73
	5832 5833	C	LYS D LYS D	154 154	32.056 31.329	42.967 43.802	27.134 27.662	1.00	72.61
30	5834	Ň	VAL D	155	32.792	43.226	26.065	1.00 1.00	72.61 92.93
	5835	CA	VAL D	155	32.751	44.532	25.426	1.00	92.93
	5836	CB	VAL D	155	34.140	45.153	25.313	1.00	130.27
	5837 5838	CG1 CG2	VAL D VAL D	155	34.065	46.494	24.609	1.00	130.27
35	5839	C	VAL D	· 155 155	34.714 32.216	45.331 44 <i>.2</i> 75	26.689 24.040	1.00 1.00	130 <i>.2</i> 7 92.93
	5840	ŏ	VAL D	155	32.715	43.395	23,330	1.00	92.93
	5841	N	TRP D	156	31.205	45.046	23.653	1.00	158.38
	5842	CA	TRP D	156	30.579	44.860	22.358	1.00	158.38
40	5843 5844	CB CG	TRP D	156 156	31.605 32.236	44.866 46.155	21.235 21.100	1.00 1.00	243.82
	5845	CD2	TRP D	156	31.589	47.366	20.812	1.00	243.82 243.82
	5846	CE2	TRP D	156	32.575	48.376	20.781	1.00	243.82
	5847	CE3	TRP D	156	30.261	47.713	20.608	1.00	243.82
45	5848 5849	CD1 NE1	TRP D	156 156	33.550 33.771	46.428 47.767	21.198	1.00	243.82
15	5850	CZ2	TRP D	156	32.278	47. 767 49.703	21.014 20.533	1.00 1.00	243.82 243.82
	5851	CZ3	TRP D	156	29.993	49.006	20.358	1.00	243.82
	5852	CH2	TRP D	156	30.983	49.997	20.320	1.00	243.82
50	5853 5854	C O	TRP D	156	29.982	43.492	22.407	1.00	158.38
50	5855	Ň	TRP D GLN D	156 157	28.886 30.752	43.299 42.528	22.908 21.924	1.00 1.00	158.38
	5856	ĊA	GLN D	157	30.284	41.168	21.881	1.00	148.04 148.04
	5857	СВ	GLN D	157	29.612	40.948	20.533	1.00	249.45
55	5858	CG	GLN D	157	28.288	41.684	20.483	1.00	249.45
JJ	5859 5860	CD OE1	GLN D	157 157	27.435	41.306	21.676	1.00	249.45
	5861	NE2	GLN D	157 157	27.203 26.9 6 3	40.132 42.292	21.914 22.421	1.00 1.00	249.45 249.45
	5862	C	GLN D	157	31.348	40.127	22.150	1.00	148.04
60	5863	0	GLN D	157	31.140	38.936	21.912	1.00	148.04
60	5864	N	LEU D	158	32.488	40.579	22.665	1.00	85.54
	5865 5866	CA CB	LEU D	158 158	33.584 34.779	39.676 39.917	22.996 22.073	1.00 1.00	85.54 127 62
	5867	ČĞ	LEU D	158	34.714	39.361	20.649	1.00	127.62 127.62
C.F	5868	CD1	LEU D	158	36.094	38.823	20.329	1.00	127.62
65	5869	CD2	LEU D	158	33.694	38.231	20.514	1.00	127.62
	5870 5871	C O	LEU. D LEU D	158 158	34.022 33.857	39.797	24.457	1.00	85.54
	5872	Ň	ASP D	159	34.562	40.847 38,706	25.090 24.986	1.00 1.00	85.54 91.88
	5873	CA	ASP D	159	35.024	38.662	26.363	1.00	91.88
70	5874	CB	ASP D	159	34.915	37.229	26.901	1.00	249.49

	5875	CG	ASP D	159	33.518	36.644	26.743	1.00	040.40
	5876	OD1	ASP D	159	32.559	37.204	27.319	1.00 1.00	249.49
	5877	OD2	ASP D	159	33.380	35.620	26.039	1.00	249.49 249.49
	5878	C	ASP D	159	36.476	39.142	26.462	1.00	91.88
5	5879	0	ASP D	159	37.270	38.921	25.543	1.00	91.88
	5880	N	TYR D	160	36.818	39.807	27.568	1.00	90.02
	5881	CA	TYR D	160	38.179	40.298	27.785	1.00	90.02
	5882	СВ	TYR D	160	38.334	41.742	27.323	1.00	132.54
10	5883	CG	TYR D	160	37.907	41.996	25.905	1.00	132.54
10	5884	CD1	TYR D	160	36.605	42.362	25.617	1.00	132.54
	5885	CE1	TYR D	160	36.196	42.585	24.315	1.00	132.54
	5886 5887	CD2 CE2	TYR D	160	38.800	41.857	24.851	1.00	132.54
	5888	CZ	TYR D	160 160	38.405 37.101	42.075 42.437	23.539 23.278	1.00	132.54
15	5889	OH	TYR D	160	36.697	42.638	21.977	1.00 1.00	132.54
••	5890	Č.	TYR D	160	38.594	40.222	29.239	1.00	132.54
	5891	ŏ	TYR D	160	37.782	40.394	30.143	1.00	90.02 90.02
	5892	Ň	GLU D	161	39.884	39.979	29.436	1.00	92.36
	5893	CA	GLU D	161	40.492	39.862	30.750	1.00	92.36
20	5894	СВ	GLU D	161	41.247	38.536	30.815	1.00	148.75
	5895	CG	GLU D	161	42.005	38.266	32.084	1.00	148.75
	5896	CD	GLU D	161	42.398	36.810	32.189	1.00	148.75
	5897	OE1	GLU D	161	43.333	36.490	32.957	1.00	148.75
25	5898	OE2	GLU D	161	41.757	35.985	31.506	1.00	148.75
23	5899	C	GLU D	161	41.448	41.051	30.923	1.00	92.36
	5900	0 N	GLU D	161	42.157	41.424	29.985	1.00	92.36
	5901 5902	CA	SER D	162	41.450	41.655	32.110	1.00	74.96
	5903	CB	SER D	162 162	42.323 41.652	42.789	32.404	1.00	74.96
30	5904	OG OG	SER D	162	41.052	43.705 42.998	33.398 34.594	1.00	62.82
-	5905	Č	SER D	162	43.671	42.370	32.989	1.00 1.00	62.82
	5906	ŏ	SER D	162	43.876	41.208	33.354	1.00	74.96 74.96
	5907	N	GLU D	163	44.593	43.325	33.088	1.00	68.26
	5908	CA	GLU D	163	45.929	43.034	33.625	1.00	68.26
35	5909	CB	GLU D	163	46.877	44.206	33.368	1.00	242.79
	5910	CG	GLU D	163	47.352	44.338	31.925	1.00	242.79
	5911	CD	GLU D	163	48.358	43.2 66	31.540	1.00	242.79
	5912	OE1	GLU D	163	49.400	43.158	32.222	1.00	242.79
40	5913 5914	OE2	GLU D	163	48.113	42.537	30.556	1.00	242.79
40	5914 5915	C	GLU D	163	45.768	42.820	35.117	1.00	68.26
	5916	Ň	GLU D PRO D	163 164	44.970 46.511	43.504	35.751	1.00	68.26
	5917	CD	PRO D	164	47.539	41.863 40.983	35.698 35.148	1.00	51.48
	5918	CA	PRO D	164	46.359	41.659	37.137	1.00 1.00	112.85
45	5919	CB	PRO D	164	47.112	40.364	37.367	1.00	51.48 112.85
	5920	CG	PRO D	164	48.211	40.465	36.404	1.00	112.85
	5921	С	PRO D	164	46.955	42.827	37.920	1.00	51.48
	5922	0	PRO D	164	47.839	43.536	37.411	1.00	51.48
50	5923	N	LEU D	165	46.480	43.045	39.145	1.00	58.03
50	5924	CA	LEU D	165	46.988	44.134	39.944	1.00	58.03
	5925	CB	LEU D	165	46.065	45.333	39.824	1.00	67.82
	5926 5927	CG	LEU D	165	46.417	46.436	40.816	1.00	67.82
	5927 5928	CD1	LEU D	165	47.878	46.685	40.736	1.00	67.82
55	5929	CD2 C	LEU D	165 165	45.653	47.711	40.495	1.00	67.82
55	5930	ŏ	LEU D	165	47.080 46.082	43.744 43.313	41.384	1.00	58.03
	5931	Ň	ASN D	166	48.274	43.892	41.957 41.964	1.00	58.03
	5932	ĊA	ASN D	166	48.513	43.551	43.367	1.00 1.00	50.98
	5933	CB	ASN D	166	49.984	43.249	43.618	1.00	50.98 110.65
60	5934	CG	ASN D	166	50.324	41.777	43.461	1.00	110.65
	5935	OD1	ASN D	166	49.514	40.900	43.700	1.00	110.65
	5936	ND2	ASN D	166	51.557	41.517	43.077	1.00	110.65
	5937	С	ASN D	166	48.084	44.660	44.311	1.00	50.98
4 F	5938	0	ASN D	166	48.175	45.818	43.992	1.00	50.98
65	5939	N	ILE D	167	47.626	44.290	45.489	1.00	69.36
	5940	CA	ILE D	167	47.167	45.267	46.443	1.00	69.36
	5941 5942	CB CG2	ILE D	167	45.659	45.375	46.397	1.00	42.00
	5942 5943	CG2 CG1	ILE D	167	45.152	46.062	47.661	1.00	42.00
70	5 94 3	CD1	ILE D	167 167	45.241	46.105	45.129	1.00	42.00
	55-7-7	501	ILE U	107	43.748	46.402	45.115	1.00	42.00

	5945	С	ILE D	107	47 667	44.040	4		
	5946	ŏ	ile d ile d	167 167	47.557 47.366	44.842 43.682	47.833	1.00	69.36
	5947	Ň	THR D	168	48.090	45.774	48.218 48.603	1.00 1.00	69.36 69.22
_	5948	CA.	THR D	168	48.480	45.418	49.945	1.00	69.22
5	5949	CB	THR D	168	49.988	45.453	50.107	1.00	70.81
	5950 5951	OG1 CG2	THR D THR D	168	50.575	44.544	49.169	1.00	70.81
	5952	C	THR D	168 168	50.372 47.84∶	45.030 46.301	51.511	1.00	70.81
	5953	ŏ	THR D	168	47.754	47.509	50.987 50.828	1.00 1.00	69.22
10	5954	N	VAL D	169	47.387	45.670	52.051	1.00	69.22 66.57
	5955	CA	VAL D	169	46.774	46.361	53.155	1.00	66.57
	5956 5957	CB CG1	VAL D VAL D	169	45.379	45.806	53.417	1.00	62.74
	5958	CG2	VAL D VAL D	169 169	44.945 44.418	46.137 46.381	54.819	1.00	62.74
15	5959	č	VAL D	169	47.693	46.061	52.416 54.334	1.00 1.00	62.74
	5960	0	VAL D	169	47.740	44.932	54.805	1.00	66.57 66.57
	5961	N	ILE D	170	48.460	47.051	54.780	1.00	82.22
	5962 5963	CA CB	ILE D	170	49.360	46.864	55.913	1.00	82.22
20	5964	CG2	ILE D	170 170	50.599 51.201	47.738 47.504	55.759	1.00	114.31
	596 5	CG1	ILE D	170	50.232	49.218	54.406 55.860	1.00 1.00	114.31
	5966	CD1	ILE D	170	51.416	50.187	55.670	1.00	114.31 114.31
	5967	C	ILE D	170	48.613	47.237	57.189	1.00	82.22
25	5968 5969	O N	ILE D LYS D	170	47.459	47.676	57.122	1.00	82.22
	5970	CA	LYS D	171 171	49.245 48.598	47.053 47.390	58.347	1.00	108.79
	5971	CB	LYS D	171	48.214	46.117	59.620 60.360	1.00 1.00	108.79
	5972	CG	LYS D	171	49.380	45.194	60.614	1.00	188.56 188.56
30	5973	CD	LYS D	171	48.910	43.762	60.800	1.00	188.56
30	5974 5975	CE NZ	LYS D LYS D	171	47.946	43.624	61.976	1.00	188.56
	5976	C	LYS D	171 171	47.459 49.453	42.220 48.270	62.130	1.00	188.56
	5977	ŏ	LYS D	171	48.981	48.761	60.524 61.549	1.00 1.00	108.79
25	5978	C1	NAG D	221	40.344	65.629	28.022	1.00	108.79 249.77
35	5979	C2	NAG D	221	39.010	64.922	27.810	1.00	249.77
	5980 5981	N2 C7	NAG D NAG D	221	39.203	63.489	27.903	1.00	249.77
	5982	07	NAG D	221 221	38.191 37.073	62.705	28.261	1.00	249.77
	5983	C8	NAG D	221	38.462	63.139 61.211	28.545 28.324	1.00 1.00	249.77
40	5984	C3	NAG D	221	38.434	65.256	26.441	1.00	249.77 249.77
	5985 5986	03	NAG D	221	37.116	64.735	26.342	1.00	249.77
	5987	C4 O4	NAG D NAG D	221 221	38.404	66.763	26.173	1.00	249.77
	5988	C5	NAG D	221	38.077 39.780	66.947 67.394	24.777	1.00	249.77
45	5989	O 5	NAG D	221	40.191	67.042	26.498 27.838	1.00 1.00	249.77
	5990	C6	NAG D	221	39.770	68.913	26.439	1.00	249.77 249.77
	5991 5992	O6	NAG D	221	38.854	69.459	27.379	1.00	249.77
	5993	C1 C2	NAG D NAG D	222	37.635	68.189	24.343	1.00	233.91
50	5994	N2	NAG D	222 222	36.436 35.346	68.019 67.346	23.396	1.00	233.91
	5995	C7	NAG D	222	34.173	67.955	24.082 24.234	1.00 1.00	233.91 233.91
	5996	07	NAG D	222	33.947	69.093	23.816	1.00	233.91
	5997	C8	NAG D	222	33.082	67.183	24.963	1.00	233.91
55	5998 5999	C3 O3	NAG D NAG D	222 222	36.855	67.215	22.156	1.00	233.91
	6000	C4	NAG D	222	35.790 38.102	67.196 67.829	21.217	1.00	233.91
	6001	O4	NAG D	222	38.567	66.974	21.503 20.471	1.00 1.00	_ು3.91
	6002	C5	NAG D	222	39.211	68.020	22.542	1.00	233.91 233.91
60	6003 6004	O5	NAG D	222	38.722	68.817	23.644	1.00	233.91
00	6005	C6 O6	nag d Nag d	222 222	40.435	68.722	21.989	1.00	233.91
	6006	C1	NAG D	242	41.628 59.627	68.076 58.578	22.406	1.00	233.91
	6007	C2	NAG D	242	59.450	58.871	32.960 31.486	1.00 1.00	107.57 107.57
45	6008	N2	NAG D	242	59.010	60.232	31.316	1.00	107.57 107.57
65	6009 6010	C7	NAG D	242	59.707	61.044	30.534	1.00	107.57
	6011	O7 C8	NAG D	242	60.732	60.679	29.950	1.00	107.57
	6012	C3	NAG D NAG D	242 242	59.199 58.412	62.478	30.373	1.00	107.57
~~	6013	Q3	NAG D	242	58.316	57.932 58.138	30.887	1.00	107.57
70	6014	Ċ4	NAG D	242	58.806	56.496	29.483 31.148	1.00 1.00	107.57 107.57
					•		J TO	1.00	107.57

WO 00/26246 PCT/US99/26203

		•							
	6015	04	NAG D	242	57.728	55.629	30.752	1.00	107.57
	6016	C5	NAG D	242	59.118	56.268	32.625	1.00	107.57
	6017 6018	O5 C6 .	NAG D	242	60.064	57.236	33.114	1.00	107.57
5	6019	O6 .	NAG D NAG D	242 242	59.783	54.930	32.783	1.00	107.57
	6020	C1	NAG D	243	59.082 57.985	54.107 54.763	33.697	1.00	107.57
	6021	C2	NAG D	243	57.985 57.074	54.762 53.527	29.705	1.00	125.30
	6022	N2	NAG D	243	57.074 57.321	52.782	29.789 31.013	1.00	125.30
	6023	C7	NAG D	243	56.303	52.357	31.758	1.00	125.30
10	6024	07	NAG D	243	55.129	52.583	31.473	1.00	125.30
	6025	C8	NAG D	243	56.634	51.574	33.018	1.00 1.00	125.30
	6026	C3	NAG D	243	57.345	52.629	28.586	1.00	125.30 125.30
	6027	O3	NAG D	243	56.458	51.521	28.595	1.00	125.30
	6 028	C4	NAG D	243	57.191	53.414	27.277	1.00	125.30
15	6029	04	NAG D	243	57.612	52.582	26.156	1.00	125.30
	5030	C5	NAG D	243	58.083	54.659	27.339	1.00	125.30
	6031	O5	NAG D	243	57.744	55.459	28.483	1.00	125.30
	6032	C6	NAG D	243	57.985	55,549	26.119	1.00	125.30
20	6033 6034	O6 C1	NAG D	243	56.713	56,172	26.043	1.00	125.30
20	6035	C2	MAN D MAN D	244	56.846	52.4∠4	25.031	1.00	205.85
	6036	02	MAN D	244 244	55.417	51.844	25.171	1.00	205.85
	6037	C3	MAN D	244	54.487 55.275	52.897	25.184	1.00	205.85
	6038	03	MAN D	244	54.016	51.012	23.858	1.00	205.85
25	6039	C4	MAN D	244	55.586	50.380 51.831	23.757 22.569	1.00	205.85
	6040	Ö4	MAN D	244	55.419	51.015	21.411	1.00	205.85
	6041	C5	MAN D	244	57.054	52.305	22.669	1.00 1.00	205.85
	6042	O5	MAN D	244	57.244	53.154	23.833	1.00	205.85
	6043	C6	MAN D	244	57.597	52.991	21.412	1.00	205.85 205.85
30	6044	O6	MAN D	244	57.221	54.349	21.357	1.00	205.85
	6045	C1	NAG D	250	45.992	76.510	37.679	1.00	248.68
	6046	C2	NAG D	250	44.579	76.931	38.128	1.00	248.68
	6047	N2	NAG D	250	44.536	77.116	39.567	1.00	248.68
35	6048	C7	NAG D	250	44.384	78.333	40.083	1.00	248.68
55	6049 6050	O7 C8	NAG D	250	44.277	79.347	39.391	1.00	248.68
	6051	C3	NAG D	250	44.348	78.442	41.599	1.00	248.68
	6052	∝ ⊙3	nag d Nag d	250 250	43.573	75.849	37.715	1.00	248.68
	6053	C4	NAG D	250 250	42.252 43.682	76.265 75.570	38.034	1.00	248.68
40	6054	04	NAG D	250	42.841	75.570 74.477	36.213 35.869	1.00	248.68
	6055	C5	NAG D	250	45.139	75.244	35.834	1.00 1.00	248.68
	6056	O 5	NAG D	250	46.017	76.312	36.259	1.00	248.68
	6057	C6	NAG D	250	45.335	75.070	34.335	1.00	248.68 248.68
	6058	. O 6	NAG D	250	46.713	75.089	33.986	1.00	248.68
45	6059	Ç1	NAG D	274	63.247	69.025	55.540	1.00	209.92
	6060	C2	NAG D	274	62.953	68.056	56.695	1.00	209.92
	6061	N2	NAG D	274	61.768	68.477	57.416	1.00	209.92
	6062	C7	NAG D	274	61.053	67.585	58.098	1.00	209.92
50	6063 6064	O7 C8	NAG D	274	61.342	66.390	58.145	1.00	209.92
50	6065	င်ဒိ	NAG D NAG D	274	59.826	68.096	58.835	1.00	209.92
	6066	O3	NAG D	274 274	64.147	68.007	57.654	1.00	209.92
	6067	C4	NAG D		63.927	67.009 67.703	58.639	1.00	209.92
	6068	04	NAG D	274 274	65.443 66.552	67.703 67.817	56.893	1.00	209.92
55	6069	C5	NAG D	274	65.610	67.817 68.683	57.775	1.00	209.92
	6070	O5	PING D	274	64.452	68.631	55.725 54.865	1.00 1.00	209.92
	6071	C6	NAG D	274	66.820	68.373	54.862	1.00	209.92
	6072	O6	NAG D	274	66.810	69.142	53.667	1.00	209.92 209.92
	6073	C1	NAG D	335	32.860	53.594	38.525	1.00	187.23
60	6074	C2	NAG D	335	32.657	54.924	39.281	1.00	187.23
	6075	N2	NAG D	335	32.302	54.604	40.651	1.00	187.23
	6076	C7	NAG D	335	33.089	54.970	41.656	1.00	187.23
	6077	07	NAG D	335	34.133	55.601	41.498	1.00	187.23
65	6078	C8	NAG D	335	32.640	54.583	43.054	1.00	187.23
O)	6079	C3	NAG D	335	31.561	55.826	38.691	1.00	187.23
	6080	O3	NAG D	335	31.736	57.155	39.169	1.00	187.23
	6081 6082	64	NAG D	335	31.606	55.833	37.168	1.00	187.23
	6083	O4 C5	NAG D	335	30.534	56.616	36.658	1.00	187.23
70	6084	O5	nag d Nag d	335 335	31.498	54.394	36.668	1.00	187.23
			mad D	555	32.666	53.657	37.089	1.00	187.23

	6085 6086	C6 O6	NAG D NAG D	335 335	31.442 30.243	54.317 53.705	35.144 34.692	1.00 1.00	187.23 187.23
	6087	C1	NAG D	340	36.447	48.280	60.935	1.00	247.88
_	6088	C2 ·	NAG D	340	37.563	48.157	61.941	1.00	247.88
5	6089	N2	NAG D	340	38.786	47.736	61.296	1.00	247.88
	6090	C7	NAG D	340	39.907	48.420	61.502	1.00	247.88
	6091 6092	O7 C8	NAG D	340	39.959	49.402	62.248	1.00	247.88
	6093	C3	nag d Nag d	340	41.160	47.954	60.781	1.00	247.88
10	6094	03	NAG D	340 340	37.180 38.213	47.173 47.101	63.025	1.00	247.88
. •	6095	C4	NAG D	340	35.881	47.101 47.637	64.002 63.677	1.00	247.88
	6096	04	NAG D	340	35.406	46.605	64.547	1.00 1.00	247.88
	6097	C5	NAG D	340	34.778	47.988	62.613	1.00	247.88
	6098	O5	NAG D	340	35.305	48.810	61.587	1.00	247.88 247.88
15	6099	C6	NAG D	340	33.729	48.850	63.239	1.00	247.88
	6100	O 6	NAG D	340	33.003	49.565	62.297	1.00	247.88
	6101	C1	NAG D	366	51.975	40.156	42.859	1.00	179.92
	6102	C2	NAG D	366	53.015	40.152	41.753	1.00	179.92
20	6103	N2	NAG D	366	52.433	40.714	40.551	1.00	179.92
20	6104	C7 O7	NAG D	366	52.553	42.013	40.303	1.00	179.92
	6105 6106	C8	NAG D	366	53.160	42.786	41.048	1.00	179.92
	6107	čš	NAG D NAG D	366 366	51.908 53.483	42.532	39.029	1.00	179.92
	6108	03	NAG D	366	54.558	38.733 38.758	41.488	1.00	179.92
25	6109	C4	NAG D	366	53.939	38.053	40.562 42.783	1.00	179.92
	6110	04	NAG D	366	54.150	36.651	42.763	1.00 1.00	179.92
	6111	C5 -	NAG D	366	52.883	38.216	43.899	1.00	179.92
	6112	O 5	NAG D	366	52.522	39.602	44.056	1.00	179.92 179.92
	6113	C6	NAG D	366	53.364	37.740	45.257	1.00	179.92
30	6114	O 6	NAG D	366	52.346	37.880	46.242	1.00	179.92
	6115	C1	NAG D	367	55.386	36.120	42.861	1.00	249.52
	6116	C2	NAG D	367	55.270	34.606	43.041	1.00	249.52
	6117	N2	D DAN	367	54.288	34.289	44.061	1.00	249.52
35	6118	C7	NAG D	367	53.121	33.757	43.710	1.00	249.52
33	6119 6120	O7 C8	nag d Nag d	367	52.823	33.510	42.539	1.00	249.52
	6121	ဖ ိ	NAG D	367 367	52.132	33.450	44.825	1.00	249.52
	6122	og Og	NAG D	367	56.643 56.568	34.041 32.629	43.413	1.00	249.52
	6123	C4	NAG D	367	57.655	34.411	43.535 42.327	1.00 1.00	249.52
40	6124	04	NAG D	367	58.951	33.973	42.709	1.00	249.52
	6125	C5	NAG D	367	57.659	35.931	42.108	1.00	249.52 249.52
	6126	O5	NAG D	367	56.321	36.405	41.807	1.00	249.52
	6127	C6	NAG D	367	58.553	36.343	40.953	1.00	249.52
45	6128	Q6	NAG D	367	57.795	36.836	39.858	1.00	249.52
45	6129	CB	LYS E	4	12.130	63.790	1.727	1.00	161.25
	6130	ca	LYS E	4	10.709	63.348	1.434	1.00	181.25
	6131 6132	CD CE	LYS E	4	9.964	63.056	2.721	1.00	181.25
	6133	NZ	LYS E Lys e	4	8.534	62.631	2.447	1.00	181.25
50	6134	C	LYS E	4 4	7.791 12.157	62.349 65.360	3.709	1.00	181.25
	6135	ŏ	LYS E	4	11.355	65.259 65.991	-0.281	1.00	249.30
	6136	Ň	LYS E	4	14.286	64.661	0. 294 0.874	1.00 1.00	249.30
	6137	CA	LYS E	4	12.924	64.186	0.485	1.00	249.30
	6138	N	PRO E	5	12.400	65.365	-1.597	1.00	249.30 120.68
55	6139	CD	PRO E	5	13.529	64.775	-2.329	1.00	144.78
	6140	CA	PRO E	5	11.713	66.365	-2.422	1.00	120.68
	6141	CB	PRO E	5	12.699	66.600	-3.566	1.00	144.78
	6142	ÇG	PRO E	5	13.298	65.263	-3.751	1.00	144.78
60	6143	C	PRO E	5	10.345	65.902	-2.912	1.00	120.68
OU	6144	0	PRO E	5	10.065	64.705	-2.963	1.00	120.68
	6145 6146	N CA	LYS E	6	9.489	66.856	-3.263	1.00	141.31
	6146 6147	CA CB	LYS E LYS E	6	8.153	66.534	-3.743	1.00	141.31
	6148	CG	LYS E	6	7.152 5.747	66.622	-2.590	1.00	196.63
65	6149	CD	LYS E	6 6	5.747 4.834	66.182	-2.959	1.00	196.63
	6150	CE	LYS E	6	4.834 3.443	66.110 65.633	-1.741	1.00	196.63
	6151	NZ	LYS E	6	2.521	65.623 65.453	-2.137	1.00	196.63
	6152	C	LYS E	6	7.735	67.460	-0.973 -4.883	1.00	196.63
	6153	ŏ	LYS E	6	7.596	68.669	-4.698	1.00 1.00	141.31
70	6154	N	VAL E	7	7.526	66.874	-6.059	1.00	141.31 81.07
						•			31.07

	6155 6156 6157	CA CB CG1	VAL E VAL E VAL E	7. 7 7	7.145 7.188 6.965	67.622 66.745 67.610	-7.259 -8.530 -9.757	1.00 1.00 1.00	81.07 76.53
5	6158 6159	CG2 C	VAL E VAL E	7 7	8.488 5.738	66.003 68.181	-8.626 -7.212	1.00	76.53 76.53 81.07
	6160 6161 6162	O N CA	VAL E SER E SER E	7 8 8	4.778 5.606	67.426 69.498	-7.151 -7.268	1.00 1.00	81.07 146.33
10	6163 6164	CB OG	SER E SER E	8	4.287 4.268 5.288	70.111 71.325 72.253	-7.266 -6.332 -6.669	1.00 1.00 1.00	146.33 208.51
	6165 6166	C O	SER E	8 8	3.948 4.829	70.536 70.605	-8.692 -9.548	1.00 1.00	208.51 146.33 146.33
15	6167 6168 6169	N CA CB	LEU E LEU E	9 9 9	2.671 2.221	70.806 71.236	-8.946 -10.269	1.00 1.00	130.86 130.86
	6170 6171	CG CD1	LEU E	9 9	1.358 1.921 1.089	70.166 68.783 68.115	-10.929 -11.217 -12.291	1.00 1.00 1.00	129.83 129.83 129.83
20	6172 6173	CD2	LEU E	9 9	3.337 1.393	68.911 72.513	-11.693 -10.206	1.00 1.00	129.83 130.86
20	6174 6175 6176	O N CA	LEU E ASN E ASN E	9 10 10	0.783 1.356 0.572	72.822 73.248	-9.184 -11.311	1.00 1.00	130.86 238.98
	6177 6178	CB CG	ASN E ASN E	10 10	1.327 0.451	74.473 75.629 76.844	-11.372 -10.726 -10.530	1.00 1.00 1.00	238.98 166.05 166.05
25	6179 6180	OD1 ND2	ASN E	10 10	-0.489 0.745	76.822 77.911	-9.737 -11.263	1.00	166.05 166.05
	6181 6182 6183	C O N	ASN E ASN E PRO E	10 10 11	0.235 1.112 -1.053	74.821 75.191 74.715	-12.817 -13.598	1.00 1.00	238.98 238.98
30	6184 6185	CD CA	PRO E	11 11	-1.439 -2.214	74.713 74.939 74.304	-13.195 -14.595 -12.392	1.00 1.00 1.00	125.56 163.67 125.56
	6186 6187 6188	CB CG C	PRO E	11	-3.341 -2.903	74.258 75.247	-13.429 -14.467	1.00 1.00	163.67 163.67
35	6189 6190	00 0	PRO E PRO E PRO E	11 11 12	-2.053 -1.179 -2.887	72.952 72.163 72.668	-11.676 -12.027 -10.663	1.00	125.56 125.56
	6191 6192	CD CA	PRO E PRO E	12 12	-3.978 -2.826	73.517 71.412	-10.138 -9.907	1.00 1.00 1.00	68.14 156.84 68.14
40	6193 6194 6195	CG C	PRO E	12 12	-3.863 -4.037	71.600 73.077	-8.802 -8.709	1.00 1.00	156.84 156.84
	6196 6197	0 N	PRO E PRO E TRP E	12 12 13	-3.214 -2.835 -3.987	70.234 69.084 70.547	-10.814 -10.562 -11.857	1.00 1.00 1.00	68.14 68.14
45	6198 6199	CA CB	TRP E	13 13	-4.488 -5.267	69.551 70.231	-12.800 -13.916	1.00	90.03 90.03 120.89
	6200 6201 6202	CG CD2 CE2	TRP E	13 13 13	-6.235 -7.024	71.215 71.111	-13.407 -12.227	1.00 1.00	120.89 120.89
50	6203 6204	CE3 CD1	TRP E	13 13	-7.750 -7.191 -6.509	72.310 70.121 72.430	-12.102 -11.255 -13.945	1.00 1.00 1.00	120.89 120.89 120.89
	6205 6206	NE1 CZ2	TRP E	13 13	-7.418 -8.627	73.100 72.548	-13.167 -11. 04 2	1.00	120.89 120.89
55	6207 6208 6209	CZ3 CH2 C	TRP E TRP E TRP E	13 13 13	-8.065 -8.768	70.359 71.561	-10.204 -10.104	1.00	120.89 120.89
	6210 6211	O N	TRP E	13 14	-3.377 -2.479 -3.443	68.727 69.264 67.415	-13.398 -14.031 -13.192	1.00 1.00 1.00	90.03 90.03 80.76
60	6212 6213 6214	CA CB	ASN E	14 14	-2.431 -1.883	66.516 65.579	-13. 72 0 -12.622	1.00 1.00	80.76 101.28
00	6215 6216	CG OD1 ND2	ASN E ASN E ASN E	14 14 14	-2.896 -3.979 -2.542	64.571 64.933 63.293	-12.133 -11.674	1.00 1.00	101.28 101.28
<i></i>	6217 6218	CO	ASN E ASN E	14 14	-2.917 -2.303	65.715 64.709	-12.211 -14.921 -15.288	1.00 1.00 1.00	101.28 80.76 80.76
65	6219 6220 6221	N CA CB	ARG E	15 15	-4.026 -4.554	66.154 65.520	-15.523 -16. 7 32	1.00 1.00	74.26 74.26
	6222 6223	CG	ARG E ARG E ARG E	15 15 15	-5.855 -5.888 -7.202	64.779 63.996 63.278	-16.490 -15.236 -15.142	1.00	82.67 82.67
70	6224	NE	ARG E	15	-7.314	62.199	-15.142 -16.114	1.00 1.00	82.67 82.67

	6225 6226	CZ NH1	ARG E	15	-8.470	61.801	-16.627	1.00	82.67
	6227	NH2	ARG E	15	-9.582	62.415	-16.260	1.00	82.67
	6228	C .	ARG E	15 15	-8.523 -4.860	60.784 66.730	-17.483	1.00	82.67
5	6229	ŏ	ARG E	15	-5.753	67.509	-17.570 -17.232	1.00	74.26
•	6230	Ň	ILE E	16	-4.116	66.920	-18.647	1.00 1.00	74.26
	6231	CA	ILE E	16	-4.363	68.085	-19.460	1.00	117.86
	6232	СВ	ILE E	16	-3.213	69.070	19.378	1.00	11 7.8 6 89. 6 8
	6233	CG2	ILE E	16	-3.128	69.663	-17.980	1.00	89.68
10	6234	CG1	ILE E	16	-1.917	68.359	-19.758	1.00	89.68
	6235	CD1	ILE E	16	-0.707	69.252	-19.676	1.00	89.68
	6236	С	ILE E	16	-4.589	67.773	-20.909	1.00	117.86
	6237	0	ILE E	16	-4.302	66.678	-21.390	1.00	117.86
16	6238	N	PHE E	17	-5.103	68.784	-21.591	1.00	150.96
15	6239	CA	PHE E	17	-5.417	68.746	-23.003	1.00	150.96
	6240	CB	PHE E	17	-6.466	69.815	-23.287	1.00	92.59
	6241 6242	CG	PHE E	17	-7.872	69.337	-23.168	1.00	92.59
	6243	CD1 CD2	PHE E PHE E	17 17	-8.846	70.151	-22.597	1.00	92.59
20	6244	CE1	PHE E	17	-8.251 -10.193	68.120 69.757	-23.724	1.00	92.59
20	6245	CE2	PHE E	17	-9.588	67.717	-22.577 -23.711	1.00	92.59
	6246	CZ	PHE E	17	-10.567	68.546	-23.141	1.00 1.00	92.59
	6247	č	PHE E	17	-4.169	69.021	-23.835	1.00	92.59
	6248	Ŏ	PHE E	17	-3.184	69.562	-23.333	1.00	150.96 150.96
25	6249	Ň	LYS E	18	-4.222	68.665	-25.112	1.00	145.64
	6250	CA	LYS E	18	-3.099	68.891	-26.010	1.00	145.64
	6251	CB	LYS E	18	-3.370	68.206	-27.350	1.00	192.00
	6252	CG	LYS E	18	-2.210	68.241	-28.329	1.00	192.00
	6253	CD	LYS E	18	-2.457	67.244	-29.441	1.00	192.00
30	6254	CE	LYS E	18	-1.359	67.245	-30.495	1.00	192.00
	6255	NZ	LYS E	18	-1.218	68.567	-31.1 6 5	1.00	192.00
	6256	C	LYS E	18	-2.878	70.388	-26.224	1.00	145.64
	6257	0	LYS E	18	-3.814	71.129	-26.517	1.00	145.64
35	6258	N	GLY E	19	-1.638	70.835	-26.061	1.00	249.22
33	6259 6260	CA C	GLY E	19	-1.339	72.237	-26.278	1.00	249.22
	6261	ŏ	GLY E	19 19	-1.364	73.144	-25.065	1.00	249.22
	6262	Ň	GLU E	20	-0.954 -1.837	74.298 72.648	-25.156 -23.930	1.00	249.22
	6263	CA	GLU E	20	-1.882	73.481	-22.732	1.00 1.00	144.61
40	6264	CB	GLU E	20	-2.930	72.929	-21.759	1.00	144.61 147.82
	6265	CG	GLU E	20	-4.288	72.690	-22.425	1.00	147.82
	6266	CD	GLU E	20	-5.371	72.257	-21.449	1.00	147.82
	6267	OE1	GLU E	20	-5.166	71.259	-20.729	1.00	147.82
	6268	OE2	GLU E	20	-6.435	72.910	-21.411	1.00	147.82
45	6269	Ç	GLU E	20	-0.501	73.546	-22.071	1.00	144.61
	6270	0	GLU E	20	0.412	72.815	-22.466	1.00	144.61
	6271	N.	ASN E	21	-0.335	74.432	-21.089	1.00	165.65
	6272	CA	ASN E	21	0.951	74.549	-20.407	1.00	165.65
50	6273 6274	CB	ASN E	21	1.551	75. 95 3	-20.547	1.00	216.79
50	6275	CG OD1	ASN E ASN E	<u> </u>	1.361	76.551	-21.918	1.00	216.79
	6276	ND2	ASN E	21 21	1.528	75.886	-22.943	1.00	216.79
	6277	C	ASN E	21	1.027	77.836 74.248	-21.921	1.00	216.79
	6278	ŏ	ASN E	21	0.837 -0.147	74.602	-18.917	1.00	165.65
55	6279	Ň	VAL E	22	1.868	73.608	-18.268 -18.380	1.00 1.00	165.65
	6280	CA	VAL E	22	1.912	73.265	-16.968	1.00	160.77 160.77
	6281	CB	VAL E	22	1.497	71.820	-16.737	1.00	158.92
	6282	CG1	VAL E	22	2.481	70.881	-17.426	1.00	158.92
	6283	CG2	VAL E	22	1.448	71.543	-15.256	1.00	158.92
60	6284	С	VAL E	22	3.342	73.442	-16.467	1.00	160.77
	6285	0	VAL E	22	4.306	73.287	-17.229	1.00	160.77
	6286	N	THR E	23	3.478	73.743	-15.180	1.00	119.61
	6287	CA	THR E	23	4.789	73.972	-14.581	1.00	119.61
65	6288	CB	THR E	23	4.862	75.412	-14.037	1.00	249.32
UJ	6289	OG1	THR E	23	4.505	76.335	-15.075	1.00	249.32
	6290	CG2	THR E	23	6.255	75.728	-13.537	1.00	249.32
	6291 6292	C	THR E	23	5.089	73.004	-13.434	1.00	119.61
	6293	N	LEU E	23 24	4.291	72.881	-12.515	1.00	119.61
70	6294	CA	LEU E	24 24	6.233 6.556	72.326 71.307	-13.467	1.00	105.17
. •		J A		47	0.555	71.397	-12.387	1.00	105.17

		CD	LEU E	24	7.032	70.045	-12.922	1.00	144.47
	6295	CB			6.394	69.466	-14.178	1.00	144.47
	6296	CG	LEU E	24		68.008	-14.314	1.00	
	6297	CD1	LEU E	24	6.782	_			144.47
	6298	CD2	LEU E	24	4.904	69.607	-14.118	1.00	144.47
5	6299	С	LEU E	24	7.635	71.944	-11.482	1.00	105.17
_	6300	0	LEU E	24	8.814	71.943	-11.821	1.00	105.17
	6301	Ň	THR E	25	7.238	72.386	-10.306	1.00	95.95
	6302	ČA	THR E	25	8.206	72.926	-9.380	1.00	95.95
		CB	THR E	25	7.552	74.012	-8.528	1.00	178.12
10	6303		THR E	25	6.961	74.986	-9.397	1.00	178.12
10	6304	OG1					-7. 63 9	1.00	178.12
	6305	CG2	THR E	25	8.578	74.689			
	6306	С	THR E	25	8.786	71.833	-8.486	1.00	95.95
	6307	0	THR E	25	8.062	70.964	-8.004	1.00	95.95
	6308	Ň	CYS E	26	10.098	71.858	-8.279	1.00	175.10
15	6309	CA	CYS E	26	10.709	70.859	-7.421	1.00	175.10
13			CYS E	26	10.598	71.335	-5.991	1.00	175.10
	6310	C				72.518	-5.698	1.00	175.10
	6311	0	CYS E	26	10.769				
	6312	CB	CYS E	26	12.178	70.637	-7.771	1.00	230.60
	6313	SG	CYS E	26	12.906	69.220	-6.890	1.00	230.60
20	6314	N	ASN E	27	10.293	70.392	-5.114	1.00	159.04
	6315	CA	ASN E	27	10.141	70.641	-3.696	1.00	159.04
	6316	CB	ASN E	27	10.980	69.628	-2,940	1.00	118.85
•			ASN E	27	10.546	69.486	-1.511	1.00	118.85
	6317	CG				69.537	-1.211	1.00	118.85
~ -	6318	OD1	ASN E	27	9.351				
25	6319	ND2	ASN E	27	11.506	69.298	-0.613	1.00	118.85
	6320	С	ASN E	27	10.502	72.054	-3.237	1.00	159.04
	6321	0	ASN E	27	11.646	72.331	-2.882	1.00	159.04
	6322	Ñ	GLY E	28	9.516	72.944	-3.238	1.00	225.84
	6323	CA	GLY E	28	9.750	74.315	-2.824	1.00	225.84
30			GLY E	28	8.487	75.101	-3.091	1.00	225.84
30	6324	C				75.153	-4.227	1.00	225.84
	6325	0	GLY E	28	8.021				
	6326	N	ASN E	29	7.929	75.722	-2.059	1.00	249.43
	6327	CA	ASN E	29	6.693	76.466	-2.228	1.00	249.43
	6328	CB	ASN E	29	6.026	76.682	-0.870	1.00	249.43
35	6329	CG	ASN E	29	4.607	77.193	-0.996	1.00	249.43
55	6330	OD1	ASN E	29	3.999	77.145	-2,066	1.00	249.43
	6331	ND2	ASN E	29	4.067	77.674	0.104	1.00	249.43
				29	6.820	77.799	-2.962	1.00	249.43
	6332	Ç					-3.920	1.00	249.43
4.0	6333	0	ASN E	29	6.084	78.052			
40	6334	N	ASN E	30	7.746	78.649	-2.530	1.00	249.58
	6335	CA	ASN E	30	7.903	79.952	-3.169	1.00	249.58
	6336	CB	ASN E	30	7.420	81.060	·2. 22 9	1.00	249.27
	6337	CG	ASN E	30	5.941	80.965	-1.929	1.00	249 <i>.2</i> 7
•	6338	OD1	ASN E	30	5.532	80.984	-0.770	1.00	249.27
45	6339	ND2	ASN E	30	5.128	80.865	-2.974	1.00	249.27
47			ASN E	30	9.313	80.279	-3.633	1.00	249.58
	6340	C					-4.833	1.00	249.58
	6341	0	ASN E	30	9.589	80.313			
	6342	N	PHE E	31	10.206	80.526	-2.682	1.00	249.39
	6343	CA	PHE E	31	11.567	80.882	-3.038	1.00	249.39
50	6344	CB	PHE E	31	11.939	82.212	-2.368	1.00	249.51
	6345	CG	PHE E	31	10.976	83.336	-2.673	1.00	249.51
	6346	CD1	PHE E	31	9.760	83.431	-2.003	1.00	249.51
			PHE E	31	11.275	84.285	-3.649	1.00	249.51
	6347	CD2					-2.294	1.00	249.51
ے ہے	6348	CE1	PHE E	31	8.855	84.455			
55	6349	CE2	PHE E	31	10.278	85.313	-3.949	1.00	249.51
	6350	CZ	PHE E	31	9.164	85.396	-3 <i>.2</i> 70	1.00	249.51
	6351	С	PHE E	31	12.602	79.806	-2. 72 9	1.00	249.39
	6352	0	PHE E	31	12.696	79.305	-1.605	1.00	249.39
	6353	Ň	PHE E	32	13.374	79.462	-3.760	1.00	249.36
60	6354	CA	PHE E	32	14.421	78.447	-3.678	1.00	249.36
UU			PHE E	32	14.088	77.296	-4.623	1.00	231.13
	6355	CB					-4.386	1.00	231.13
	6356	CG	PHE E	32	14.910	76.075			
	6357	CD1	PHE E	32	14.771	75.366	-3.200	1.00	231.13
	6358	CD2	PHE E	32	15.844	75.644	-5.325	1.00	231.13
65	6359	CE1	PHE E	32	15.547	74.245	-2.944	1.00	231.13
	6360	CE2	PHE E	32	16.628	74.520	-5.079	1.00	231.13
	6361	CZ	PHE E	32	16.477	73.819	-3.881	1.00	231.13
		C	PHE E	32	15.779	79.040	-4.063	1.00	249.36
	6362					80.171	-4.540	1.00	249.36
70	6363	• 0	PHE E	32	15.849				
70	6364	N	GLU E	33	16.857	.78 <i>.2</i> 77	-3.876	1.00	249.65

	6365	CA	GLU E	33	18.190	78.784	-4.212	1.00	249.65
	6366	CB	GLU E	33	19.035	78.993	-2.958	1.00	249.51
	6367 6368	CD ·	GLU E	33 33	20.347	79.715	-3.258	1.00	249.51
5	6369	OE1	GLU E	33	20.106 19.170	81.122 81.769	-3.769 -3.253	1.00	249.51
,	6370	OE2	GLU E	33	20.849	81.591	-3.253 -4.659	1.00 1.00	249.51
	6371	C	GLU E	33	19.038	77.975	-5.180	1.00	249.51 249.65
	6372	ŏ	GLU E	33	19.533	78.510	-6.173	1.00	249.65
	6373	N	VAL E	34	19.242	76.699	-4.873	1.00	249.34
10	6374	CA	VAL E	34	20.073	75.864	-5.721	1.00	249.34
	6375	CB	VAL E	34	20.055	74.399	-5.244	1.00	177.29
	6376	CG1	VAL E	34	20.927	73.540	-6 .146	1.00	177.29
	6377	CG2	VAL E	34	20.562	74.325	-3.815	1.00	177.29
1.5	6378	C	VAL E	34	19.694	75.933	-7.196	1.00	249.34
15	6379	0	VAL E	34	18.530	76.142	-7.555	1.00	249.34
	6380	N CA	SER E SER E	35	20.705	75.782	-8.040	1.00	249.49
	6381 6382	CB	SER E SER E	35 35	20.523 21.517	75.809 76. 77 9	-9.479 -10.122	1.00	249.49
	6383	OG	SER E	35 35	22.845	76.779 70.294	-10.122	1.00 1.00	217.44
20	6384	Č	SER E	35	20.763	74.397	-10.000	1.00	217.44 249.49
20	6385	ŏ	SER E	35.	20.658	74.144	-11.199	1.00	249.49
	6386	Ň	SER E	36	21.094	73.480	-9.092	1.00	249.36
	6387	CA	SER E	36	21.335	72.089	-9.464	1.00	249.36
	6388	CB	SER E	36	22.586	71.540	-8.769	1.00	172.90
25	6389	OG	SER E	36	22.371	71.370	-7.379	1.00	172.90
	6390	С	SER E	36	20.128	71.242	-9.085	1.00	249.36
	6391	0	SER E	36	20.020	70.741	-7.964	1.00	249.36
	6392	N	THR E	37	19.214	71.104	-10.036	1.00	210.16
20	6393	CA	THR E	37	18.007	70.321	-9.849	1.00	210.16
30	6394	CB	THR E	37	16.754	71.225	-9.905	1.00	202.55
	6395 6396	OG1 CG2	THR E	37 37	16.859	72.253 70.414	-8.913 -9.647	1.00	202.55
	6397	C	THR E	37 37	15.499 17.982	69.325	-9.047 -11.000	1.00 1.00	202.55
	6398	ŏ	THR E	37	18.352	69.662	-12.126	1.00	210.16 210.16
35	6399	Ň	LYS E	38	17.565	68.098	-10.718	1.00	223.06
	6400	CA	LYS E	38	17.517	67.070	-11.749	1.00	223.06
	6401	CB	LYS E	38	18.234	65.818	-11.256	1.00	249.17
	6402	CG	LYS E	38	19.660	66.069	-10.828	1.00	249.17
40	6403	CD	LYS E	38	20.313	64.794	-10.338	1.00	249.17
40	6404	CE	LYS E	38	21.769	65.032	-9.996	1.00	249.17
	6405	NZ	LYS E	38	22.436	63.783	-9.543	1.00	249.17
	6406 6407	C	LYS E	38	16.086	66.711	-12.133	1.00	223.06
	6408	Ň	TRP E	38 39	15.204 15.858	66.678 66.451	-11.281 -13.418	1.00 1.00	223.06 178.64
45	6409	CA	TRP E	39	14.530	66.068	-13.416	1.00	178.64
	6410	CB	TRP E	39	13.911	67.160	-14.768	1.00	178.88
	6411	CG	TRP E	39	13.622	68.431	-14.049	1.00	178.88
	6412	CD2	TRP E	39	12.634	68.651	-13.034	1.00	178.88
	6413	CE2	TRP E	39	12.721	70.008	-12.652	1.00	178.88
50	6414	CE3	TRP E	39	11.685	67.832	-12.407	1.00	178.88
	6415	CD1	TRP E	39	14.249	69.627	-14.235	1.00	178.88
	6416	NE1	TRP E	39	13.712	70.580	-13.400	1.00	178.88
	6417	CZ2	TRP E	39	11.896	70.564	-11.678	1.00	178.88
55	6418	CZ3	TRP E	39	10.865	68.390	-11.436	1.00	178.88
22	6419 6420	CH2 C	TRP E	39	10.978	69.744	-11.081	1.00	178.88
	6421	ŏ	TRP E	39 39	14.641 15.495	64.796 64.687	-14.710 -15.582	1.00 1.00	178.64 178.64
	6422	Ň	PHE E	40	13.771	63.838	-14,432	1.00	223.76
	6423	CA	PHE E	40	13.811	62.585	-15.159	1.00	223.76
60	6424	CB	PHE E	40	14.209	61.445	-14.223	1.00	188.15
	6425	CG	PHE E	40	15.514	61.660	-13.529	1.00	188.15
	6426	CD1	PHE E	40	15.592	62.472	-12.407	1.00	188.15
	6427	CD2	PHE E	40	16.663	61.029	-13.984	1.00	188.15
<i>(</i>	6428	CE1	PHE E	40	16.797	62.656	-11.746	1.00	188.15
65	6429	CE2	PHE E	40	17.875	61.204	-13.333	1.00	188.15
	6430	cz	PHE E	40	17.942	62.020	-12.207	1.00	188.15
	6431	C	PHE E	40	12.490	62.235	-15.834	1.00	223.76
	6432 6433	O N	PHE E	40	11.665	61.521	-15.266	1.00	223.76
70	6434	CA	HIS E	41 41	12.294 11.080	62.737 62.448	-17.048 -17.801	1.00	123.84
, 5		√ ∧	1110 6	71	11.000		-17.001	1.00	123.84

	6435	CB	HIS E	41	10.940	63.454	-18.937	1.00	124.43
	6436	ÇG	HIS E	41	9.749	63.222	-19.801	1.00	124.43
	6437	CD2	HIS E	41	9.597	63.290	-21.144	1.00	124.43
_	6438	ND1	HIS E	41	8.510	62.907	-19.289	1.00	124.43
5	6439	CE1	HIS E	41	7.645	62.789	-20.278	1.00	124.43
	6440	NE2	HIS E	41	8.280	63.016 61.013	-21.415 -18.349	1.00	124.43
	6441	C	HIS E HIS E	41 41	11.136 11.924	60.715	-18.349 -19.243	1.00 1.00	123.84
	6442 6443	O N	ASN E	42	10.298	60.132	-17.809	1.00	123.84 190.21
10	6444	CA	ASN E	42	10.269	58.717	-18.206	1.00	190.21
10	6445	CB	ASN E	42	10.027	58.550	-19.720	1.00	194.75
	6446	ČG	ASN E	42	8.588	58.839	-20.123	1.00	194.75
	6447	OD1	ASN E	42	8.009	59.813	-19.653	1.00	194.75
	6448	ND2	ASN E	42	8.017	58.019	-21.005	1.00	194.75
15	6449	С	ASN E	42	11.593	58.050	-17.826	1.00	190.21
	6450	0	ASN E	42	12.003	57.072	-18.446	1.00	190.21
	6451	N	GLY E	43	12.263	58.580	-16.806	1.00	203.91
	6452	abla	GLY E	43	13.533	58.010	-16.386	1.00	203.91
00	6453	C	GLY E	43	14.734	58.697	-17.020	1.00	203.91
20	6454	0	GLY E	43	15.758	58.901	-16.364	1.00	203.91
	6455	N	SER E	44	14.609	59.053	-18.297	1.00	245.20
	6456	CA	SER E	44	15.683	59.723	-19.030 -20.512	1.00	245.20
	6457	CB OG	SER E SER E	44 44	15.312 14.940	59.846 58.591	-20.512 -21.055	1.00 1.00	220.02 220.02
25	6458 6459	C	SER E	44	15.929	61.114	-18.452	1.00	245,20
23	6460	Ö	SER E	44	14.999	61.907	-18.326	1.00	245.20
	6461	Ň	LEU E	45	17.177	61.412	-18.101	1.00	174.49
	6462	ČA	LEU E	45	17.519	62.718	-17.541	1.00	174.49
	6463	CB	LEU E	45	19.028	62.804	-17.280	1.00	249.38
30	6464	CG	LEU E	45	19.550	64.104	-16.660	1.00	249.38
	6465	CD1	LEU E	45	18.785	64.404	-15.381	1.00	249.38
	6466	CD2	LEU E	45	21.043	63.982	-16.375	1.00	249.38
	6467	С	LEU E	45	17.095	63.834	-18.498	1.00	174.49
~-	6468	0	LEU E	45	17.140	63.672	-19.717	1.00	174.49
35	6469	N	SER E	46	16.673	64.965	-17.945	1.00	153.34
	6470	CA	SER E	46	16.247	66.094	-18.766	1.00	153.34
	6471	CB	SER E	46	15.016	66.766	-18.148	1.00	249.33
	6472	og	SER E	46	14.541	67.822 67.000	-18.971	1.00	249.33 153.34
40	6473	C	SER E SER E	46 46	17.394 18.345	67.088 66.994	-18.845 -18.072	1.00 1.00	153.34
40	6474 6475	0 N	GLU E	46 47	17.310	68.043	-19.768	1.00	221.85
	6476	CA	GLU E	47	18.371	69.035	-19.903	1.00	221.85
	6477	CB	GLU E	47	18.589	69.401	-21.384	1.00	249.45
	6478	ČĞ	GLU E	47	18.515	68.232	-22.369	1.00	249.45
45	6479	CD	GLU E	47	18.351	68.687	-23.823	1.00	249.45
	6480	OE1	GLU E	47	17.207	68.973	-24.239	1.00	249.45
	6481	OE2	GLU E	47	19.372	68.774	-24.540	1.00	249.45
	6482	С	GLU E	47	18.128	70.317	-19.081	1.00	221.85
50	6483	0	GLU E	47	18.974	71.207	-19.091	1.00	221.85
50	6484	N .	GLU E	48	16.993	70.438	-18.387	1.00	204.14
	6485	CA	GLU E	48	16.775	71.643	-17.573	1.00	204.14
	6486	СВ	GLU E	48	15.275	71.939	-17.355	1.00	206.52
	6487	CG	GLU E	48	14.973	73.087	-16.352	1.00	206.52
55	6488 6489	CD OE1	GLU E GLU ::	48 48	15.418	74.469 74.995	-16.₽ <i>2</i> 3 -17.778	1.00 1.00	206.52 206.52
25	6490	OE2	GLU E	46 48	14.812 16.370	75.032	-16.236	1.00	206.52
	6491	C	GLU E	48	17.471	71.443	-16.221	1.00	204.14
	6492	ŏ	GLU E	48	17.724	70.311	-15.798	1.00	204.14
	6493	Ň	THR E	49	17.803	72.545	-15.556	1.00	206.12
60	6494	ĊA	THR E	49	18.472	72.476	-14.266	1.00	206.12
	6495	СВ	THR E	49	19.947	72.928	-14.386	1.00	224.40
	6496	OG1	THR E	49	20.006	74.247	-14.942	1.00	224.40
	6497	CG2	THR E	49	20.721	71. 97 2	-15.288	1.00	224.40
	6498	С	THR E	49	17.747	73.335	-13 <i>.2</i> 33	1.00	206.12
65	6499	0	THR E	49	17.781	73.043	-12.035	1.00	206.12
	6500	N	ASN E	50	17.081	74.388	-13.702	1.00	231.11
	6501	CA	ASN E	50	16.330	75.2 7 2	-12.819	1.00	231.11
	6502	CB	ASN E	50	15.602	76.349	-13.640	1.00	176.85
70	6503	CG	ASN E	50	15.085	77.491	-12.783	1.00	176.85
70	6504	OD1	ASN E	50	14.962	77.346	-11.568	1.00	176.85

	6505	ND2	ASN E	50	14.770	78.622	-13.410	1.00	170.05
	6506	C	ASN E	50	15.316	74.396	-12.076		176.85
	6507	Ŏ	ASN E	50	14.884	73.368 ·		1.00	231.11
	6508	Ň.	SER E	51			-12.597	1.00	231.11
5	6509	CA			14.942	74.792	-10.863	1.00	235.89
,			SER E	51	13.985	74.015	-10.077	1.00	235.89
	6510	CB	SER E	51	13.895	74.561	-8.645	1.00	153.05
	6511	OG.	SER E	51	13.254	75.826	-8.609	1.00	153.05
	6512	С	SER E	51	12.587	73.995	-10.696	1.00	235.89
	6513	0	SER E	51	11.765	73.145	-10.358	1.00	
10	6514	N	SER E	52	12.314	74.932	-11.597		235.89
	6515	CA	SER E	52	11.009			1.00	154.90
	6516	CB	SER E			74.997	-12.245	1.00	154.90
				52	10.435	76.415	-12.157	1.00	199.68
	6517	OG	SER E	52	10.195	76.786	-10.809	1.00	199.68
16	6518	С	SER E	52	11.109	74.569	-13.700	1.00	154.90
15	6519	0	SER E	52	11.656	75.288	-14.538	1.00	154.90
	6520	N	LEU E	53	10.582	73.385	-13.985	1.00	130.79
	6521	CA	LEU E	53	10.590	72.827	-15.332	1.00	
	6522	СВ	LEU E	53	10.833	71.315			130.79
	6523	ČĞ	LEU E	53			-15.264	1.00	134.25
20	6524	CD1			10.394	70.457	-16.457	1.00	134.25
20			LEU E	53	10.802	71.095	-17.779	1.00	134.25
	6525	CD2	LEU €	53	10.999	69.065	-16.304	1.00	134.25
	6526	С	LEU E	53	9.271	73.112	-16.044	1.00	130.79
	6527	0	LEV E	53	8.279	72.435	-15.810	1.00	130.79
	6528	N	ASN E	54	9.258	74.109	-16.920	1.00	
25	6529	CA	ASN E	54	8.031	74.440			200.88
	6530	CB	ASN E	54			-17.632	1.00	200.88
	6531	CG			8.095	75.864	-18.181	1.00	249.13
			ASN E	54	7.990	76.907	-17.096	1.00	249.13
	6532	OD1	ASN E	54	7.029	76.923	-16.328	1.00	249.13
20	6533	ND2	ASN E	54	8.975	77. 79 0	-17.026	1.00	249.13
30	6534	С	ASN E	54	7.719	73.486	-18.771	1.00	200.88
	6535	0	ASN E	54	8.589	72.769	-19.265	1.00	200.88
	6536	N	ILE E	55	6.453	73.481	-19.168	1.00	
	6537	CA	ILE E	55	5.985	72.657			204.06
	6538	CB	ILE E	55			-20.269	1.00	204.06
35	6539	CG2			5.212	71.417	-19.770	1.00	202.84
55				55	4.367	70.839	-20.896	1.00	202.84
	6540	CG1	ILE E	55	6.205	70.376	-19.246	1.00	202.84
	6541	CD1	ILE E	5 5	5.569	69.111	-18.716	1.00	202.84
	6542	С	ILE E	55	5.065	73.547	-21.080	1.00	204.06
	6543	0	ILE E	55	4.086	74.074	-20.559	1.00	204.06
40	6544	N	VAL E	56	5.395	73.739	-22.349	1.00	
	6545	CA	VAL E	56	4.580	74.585			244.52
	6546	СВ	VAL E	56			-23.202	1.00	244.52
	6547	CG1	VAL E		5.458	75.494	-24.072	1.00	219.78
	6548			56	4.629	76.643	-24.618	1.00	219.78
45		CG2	VAL E	56	6.622	76.026	-23.246	1.00	219.78
43	6549	Ç	VAL E	56	3.711	73.696	-24.073	1.00	244.52
	6550	0	VAL E	56	3.545	72.522	-23.758	1.00	244.52
	6551	N	ASN E	57	3.160	74.247	-25.152	1.00	153.88
	6552	CA	ASN E	57	2.290	73.486	-26.047	1.00	
	6553	CB	ASN E	57	2.564	73.854	-27.506		153.88
50	6554	CG	ASN E	57	2.105	75.254		1.00	249.23
	6555	OD1	ASN E				-27.843	1.00	249.23
	6556			57	0.954	75.617	-27.601	1.00	249.23
		ND2	ASN E	57	3.003	76.051	-28.404	1.00	249.23
	6557	Ç	ASN E	57	2.438	71.983	-25.847	1.00	153.88
بے ہے	6558	0	ASN E	57	3.263	71.323	-26.489	1.00	153.88
55	6559	N	ALA E	58	1.624	71.458	-24.936	1.00	183.15
	6560	CA	ALA E	58	1.638	70.047	-24.587		
	6561	CB	ALA E	58	0.552	69.763		1.00	183.15
	6562	Č	ALA E	58			-23.565	1.00	127.72
	6563	ŏ			1.492	69.103	-25.766	1.00	183.15
60			ALA E	58	0.486	69.115	-26.474	1.00	183.15
oo	6564	N.	LYS E	59	2.510	68.281	-25. 968	1.00	111.87
	6565	CA	LYS E	59	2.495	67. 29 3	-27.035	1.00	111.87
	656 6	CB	LYS E	59	3.816	67.338	-27.815	1.00	249.40
	6567	CG	LYS E	59	4.115	68.702	-28.436	1.00	249.40
_	6568	CD	LYS E	59	5.489	68.753	-29.090		
65	6569	CE	LYS E	59	5.764			1.00	249.40
	6570	NZ	LYS E			70.129	-29.691	1.00	249.40
	6571			59 50	7.117	70.219	-30.310	1.00	249.40
		C	LYS E	59	2.319	65. 94 2	-26.334	1.00	111.87
	6572	0	LYS E	59	2.824	65.746	-25.226	1.00	111.87
70	6573	N	PHE E	60	1.597	65.020	-26.960	1.00	223.03
70	6574	CA	PHE E	60	1.368	63.703	-26.366	1.00	223.03
						•			حدی.س

	6575	СВ	PHE E	60	0.846	62.744 63.120	-27.427 -27.953	1.00 1.00	249.06
	6576	CG	PHE E	60	-0.496 0.976	62.774	-27.953 -29.237	1.00	249.06
	6577	CD1	PHE E PHE E	60 60	-0.876 -1.390	63.823	-25.237 -27.155	1.00	249.06 249.06
5	6578	CD2 [*] CE1	PHE E	60	-2.124	63.119	-29.727	1.00	249.06
3	6579 6580	CE2	PHE E	60	-2.640	64.176	-27.633	1.00	249.06
	6581	CZ	PHE E	60	-3.010	63.822	-28.922	1.00	249.06
	6582	Č.	PHE E	60	2.610	63.115	-25.720	1.00	223.03
	6583	ŏ	PHE E	60	2.520	62.404	-24.721	1.00	223.03
10	6584	Ň	GLU E	61	3.771	63.417	-26.296	1.00	190.77
	6585	CA	GLU E	61	5.044	62.917	-25.783	1.00	190.77
	6586	CB	GLU E	61	6.196	63.299	-26.718	1.00	249.27
	6587	CG	GLU E	61	6.096	62.728	-28.116	1.00	249.27
	6588	CD	GLU E	61	4.851	63.190	-28.838	1.00	249.27
15	6589	OE1	GLU E	61	4.635	64.418 62.327	-28.924 -29.320	1.00 1.00	249.27 249.27
	6590	OE2	GLU E GLU E	61 61	4.090 5.357	63.449	-24.395	1.00	190.77
	6591	C	GLU E	61	6.140	62.842	-23.663	1.00	190.77
	6592 6593	N	ASP E	62	4.765	64.588	-24.040	1.00	156.70
20	6594	ČA	ASP E	62	5.006	65.174	-22.727	1.00	156.70
20	6595	CB	ASP E	62	4.489	66.613	-22.678	1.00	165.21
	6596	CG	ASP E	62	5.062	67.477	-23.792	1.00	165.21
	6597	OD1	ASP E	62	6.251	67.299	-24.133	1.00	165.21
	6598	OD2	ASP E	62	4.329	68.341	-24.320	1.00	165.21
25	6599	С	ASP E	62	4.341	64.324	-21.643	1.00	156.70
	6600	0	ASP E	62	4.711	64.394	-20.470	1.00	156.70
	6601	N	SER E	63	3.358	63.523	-22.045	1.00	140.02
	6602	CA	SER E	63	2.672	62.635	-21.118	1.00	140.02
20	6603	CB	SER E	63	1.618	61.796 62.589	-21.856 -22.368	1.00 1.00	116.21 116.21
30	6604	og	SER E SER E	63 63	0.557 3.744	61.710	-20.557	1.00	140.02
	6605 6606	C O	SER E	63	4.509	61.128	-21.315	1.00	140.02
	6607	Ñ	GLY E	64	3.818	61.572	-19.243	1.00	94.90
	6608	CA	GLY E	64	4.835	60.694	-18.698	1.00	94.90
35	6609	Č.	GLY E	64	5.050	60.749	-17.195	1.00	94.90
-	6610	ŏ	GLY E	64	4.252	61.333	-16.462	1.00	94.90
	6611	N	GLU E	65	6.127	60.121	-16. 73 7	1.00	137.73
	6612	CA	GLU E	6 5	6.476	60.071	-15.323	1.00	137.73
	6613	СВ	GLU E	6 5	6.875	58.635	-14.971	1.00	170.42
40	6614	CG	GLU E	65	7.492	58.437	-13.609 -13.484	1.00 1.00	170.42 170.42
	6615	CD	GLU E	65	8.153	57.072 56.807	-13.464	1.00	170.42
	6616	OE1 OE2	GLU E GLU E	65 65	9.121 7.706	56.263	-12.644	1.00	170.42
	6617	C	GLU E	65	7.645	61.025	-15.096	1.00	137.73
45	6618 6619	ŏ	GL' E	65	8.653	60.925	-15.789	1.00	137.73
43	6620	Ň	TYR E	66	7.513	61.952	-14.147	1.00	117.13
	6621	CA	TYR E	66	8.588	62.908	-13.864	1.00	117.13
	6622	СВ	TYR E	66	8.123	64.321	-14.112	1.00	93.74
	6623	CG	TYR E	66	7.767	64.647	-15.528	1.00	93.74
50	6624	CD1	TYR E	66	6.586	64.214	-16.090	1.00	93.74
	6625	CE1	TYR E	66	6.220	64.609	-17.382	1.00	93.74
	6626	CD2	TYR E	66	8.582	65.471	-16.285	1.00	93.74 93.74
	6627	CE2	TYR E	66	8.230	65.873	-17.564 -18.110	1.00 1.00	93.74
55	6628	CZ	TYR E TYR E	66 66	7.050 6.702	65.445 65.872	-19.376	1.00	93.74
33	6629	OH C	TYR E	66 66	9.062	62.852	-12.426	1.00	117.13
	6630 6631	ŏ	TYR E	66	8.359	62.335	-11.564	1.00	117.13
	6632	Ň	LYS E	67	10.248	63.402	-12.169	1.00	125.36
	6633	ČA	LYS E	67	10.802	63.443	-10.815	1.00	125.36
60	6634	СВ	LYS E	67	11.186	62.037	-10.352	1.00	181.51
	6635	CG	LYS E	67	12.026	61.282	-11.345	1.00	181.51
	6636	CD	LYS E	67	12.264	59.876	-10.876	1.00	181.51
	6637	CE	LYS E	67	12.938	59.066	-11.956	1.00	181.51
	6638	NZ	LYS E	67	13.120	57.655	-11.522	1.00	181.51
65	6639	Ç	LYS E	67	12.014	64.362	-10.732	1.00	125.36
	6640	o.	LYS E	67	12.671	64.622	-11.737	1.00	125.36
	6641	N CA	CYS E	68	12.289	64.881 65.729	-9.541 -9.370	1.00 1.00	114.74 114.74
	6642	CA	CYS E	68 68	13.451 14.297	65.729 65.211	-9.370 -8.210	1.00	114.74
70	6643 6644	C	CYS E	68	13.824	64.428	-7.388	1.00	114.74
70	0044	J	0.0 2	00	10.024	V 1.750			

	6645	СВ	CYS E	68	13.047	67.197	-9.159	1.00	167.12
	6646	SG	CYS E	68	12.001	67.607	-7.729	1.00	167.12
	6647	N	GLN E	69	15.561	65.619	-8.180	1.00	152.39
_	6648	CA	GLN E	69	16.493	65.217	-7.139	1.00	152.39
5	6649	CB	GLN E	69	17.120	63.861	-7.482	1.00	180.76
	6650	CG	GLN E	69	18.398	63.553	-6.725	1.00	180.76
	6651	CD	GLN E	69	19.065	62.274	-7.191	1.00	180.76
	6652 6653	OE1 NE2	GLN E GLN E	69 69	19.315 19.364	62.089 61.386	-8.383 -6.250	1.00 1.00	180.76
10	6654	C	GLN E	69	17.566	66.292	-0.250 -7.067	1.00	180.76
10	6655	ŏ	GLN E	69	17.822	66.998	-8.048	1.00	152.39 152.39
	6656	Ň	HIS E	70	18.186	66.429	-5.902	1.00	249.25
	6657	CA	HIS E	70	19.226	67.429	-5.730	1.00	249.25
	6658	CB	HIS E	70	18.911	68.308	-4.519	1.00	185.63
15	6659	CG	HIS E	70	17.717	69.187	-4.713	1.00	185.63
	6660	CD2	HIS E	70	16.426	69.026	-4.338	1.00	185.63
	6661	ND1	HIS E	70	17.769	70.377	-5.406	1.00	185.63
	6662 6663	CE1 NE2	HIS E HIS E	70 70	16.560 15.729	70.915 70.114	-5.449 -4.806	1.00 1.00	185.63 185.63
20	6664	C	HIS E	70	20.605	66.806	-5.583	1.00	249.25
	6665	ŏ	HIS E	70	20.793	65.603	-5.787	1.00	249.25
	6666	N	GLN E	71	21.568	67.644	-5. 225	1.00	214.79
	6667	CA	GLN E	71	22.945	67.209	-5.061	1.00	214.79
05	6668	СВ	GLN E	71	23.787	68.387	-4.553	1.00	249.44
25	6669	CG	GLN E	71	25.227	68.347	-5.024	1.00	249.44
	6670	CD	GLN E	71	25.359	68.172	-6.526	1.00	249.44
	6671 6672	OE1 NE2	GLN E GLN E	71 71	25.049 25.815	69.077 67.001	-7.304 -6.940	1.00 1.00	249.44
	6673	C	GLN E	71	23.055	66.005	-4.119	1.00	249.44 214.79
30	6674	ŏ	GLN E	71	23.602	64.967	-4.496	1.00	214.79
	6675	N	GLN E	72	22.517	66.140	-2.906	1.00	224.12
	6676	CA	GLN E	72	22.569	65.060	-1.906	1.00	224.12
	6677	CB	GLN E	72	23.396	65.488	-0.694	1.00	220.92
25	6678	CG	GLN E	72	23.660	64.401	0.347	1.00	220.92
35	6679	CD	GLN E GLN E	72	24.599	64.863 65.260	1.460	1.00	220.92
	6680 6681	OE1 NE2	GLN E	72 72	25.746 24.108	64.811	1.224 2.684	1.00 1.00	220.92 220.92
	6682	C	GLN E	72	21.190	64.677	-1.396	1.00	224.12
	6683	ŏ	GLN E	72	20.938	64.719	-0.192	1.00	224.12
40	6684	N	VAL E	73	20.301	64.293	-2.298	1.00	249.50
	6685	CA	VAL E	73	18. 95 3	63.928	-1.899	1.00	249.50
	6686	CB	VAL E	73	18.006	65.126	-2.032	1.00	213.59
	6687	CG1	VAL E	73	16.699	64.850	-1.308	1.00	213.59
45	6688 6689	CG2 C	VAL E VAL E	73 73	18.676 18.410	66.352 62.814	-1.536 -2.776	1.00 1.00	213.59 249.50
43	6690	ŏ	VAL E	73	18.724	62.740	-3.964	1.00	249.50
	6691	Ň	ASN E	74	17.584	61.952	-2.192	1.00	249.52
	6692	CA	ASN E	74	16.994	60.858	-2.946	1.00	249.52
	6693	CB	ASN E	74	16.515	59.760	-1.994	1.00	169.17
50	6694	CG	ASN E	74	17.620	59.273	-1.081	1.00	169.17
	6695	OD1	ASN E	74	18.757	59.080	-1.522	1.00	169.17
	6696	ND2	ASN E ASN E	74 74	17,291	59.065	0.192	1.00 1.00	169.17
	6697 6698	CO	ASN E	74	15.838 14.956	61.389 62.085	-3.787 -3.283	1.00	249.52 249.52
55	6699	Ň	GLU E	75	15.870	61.071	-5.077	1.00	220.79
	6700	CA	GLU E	75	14.851	61.501	-6.025	1.00	220.79
	6701	СВ	GLU E	75	14.992	60.694	-7.316	1.00	206.72
	6702	CG	GLU E	75	15.456	59.259	-7.100	1.00	206.72
60	6703	CD	GLU E	75	15.805	58.557	-8.399	1.00	206.72
60	6704	OE1	GLU E	75	16.636	59.096	-9.159	1.00	206.72
	6705 6706	OE2	GLU E GLU E	75 75	15.254	57.465 61.414	-8.660 -5.488	1.00 1.00	206.72 220.79
	6706 6707	C O	GLU E	75 75	13.420 13.071	61.414 60.495	-5.488 -4.747	1.00	220.79 220.79
	6708	N	SER E	76	12.604	62.385	-5.885	1.00	123.65
65	6709	CA	SER E	76	11.211	62.502	-5.457	1.00	123.65
-	6710	СВ	SER E	76	10.646	63.837	-5.918	1.00	156.05
	6711	OG	SER E	76	10.583	63.854	-7.332	1.00	156.05
	6712	C	SER E	76	10.310	61.422	-5.997	1.00	123.65
70	6713	0	SER E	76	10.623	60.793	-7.006	1.00	123.65
70	6714	N	GLU E	77	9.172	61.235	-5.333	1.00	207.91

	6715	CA	GLU E	77	8.193	60.247	-5.762	1.00	207.91
	6716 6717	CB CG	GLU E	77 77	7.055 7.495	60.135 59.613	-4.744 -3.388	1.00	181.88
	6717 6718	CD.	GLU E	77	7.495 8.000	58.181	-3.440	1.00 1.00	181.88
5	6719	OE1	GLU E	77	8.281	57.684	-4.551	1.00	181.88 181.88
-	6720	OE2	GLU E	77	8.127	57.550	-2.369	1.00	181.88
	6721	С	GLU E	77	7.645	70.711	-7.103	1.00	207.91
	6722	0	GLU E	77	7.050	61.788	-7.189	1.00	207.91
10	6723	N	PRO E	78	7.857	59.919	-8.171	1.00	80.79
10	6724	CD CA	PRO E PRO E	78 70	8.716 7.390	58.718 60.237	-8.203 -9.522	1.00	240.65
	6725 6726	CB	PRO E	78 78	7.588	58.930	-9.522 -10.260	1.00 1.00	80.79 240.65
	6727	ÇG	PRO E	78	8.884	58.468	-9.399	1.00	240.65
	6728	č	PRO E	78	5.967	60.738	-9 594	1.00	80.79
15	6729	0	PRO E	78	5.145	60.436	-8.738	1.00	80.79
	6730	N	VAL E	79	5.681	61.517	-10.622	1.00	112.90
	6731	CA	VAL E	79	4.351	62.067	-10.801	1.00	112.90
	6732	CB	VAL E	79 70	4.314	63.550	-10.455	1.00	137.47
20	6733 6734	CG1 CG2	VAL E VAL E	79 79	3.032 4.403	⁻∔.176 63.715	-10.987 -8.951	1.00 1.00	137.47
20	6735	C	VAL E	79	3.978	61.908	-12.251	1.00	137.47 112.90
	6736	Ö	VAL E	79	4.737	62.312	-13.132	1.00	112.90
	6737	N	TYR E	80	2.807	61.334	-12.508	1.00	70.76
	6738	CA	TYR E	80	2.402	61.134	-13.886	1.00	70.76
25	6739	CB	TYR E	80	1.630	59.841	-14.062	1.00	159.99
	6740	CG	TYR E	80	1.595	59.441	-15.510	1.00	159.99
	6741	CD1 CE1	TYR E TYR E	80	2.763	59.078 59.714	-16.169	1.00	159.99
	6742 6743	CD2	TYR E TYR E	80 80	2.758 0.408	58.714 59.437	-17.498 -16.231	1.00 1.00	159.99 159.99
30	6744	CE2	TYR E	80	0.395	59.076	-17.589	1.00	159.99
-	6745	cz	TYR E	80	1.583	58.712	-18.206	1.00	159.99
	6746	OH	TYR E	80	1.597	58.323	-19.528	1.00	159.99
	6747	C	TYR E	80	1.562	62.238	-14.446	1.00	70.76
25	6748	0	TYR E	80	0.661	62.746	-13.795	1.00	70.76
35	6749	N CA	LEV E LEV E	81	1.838	62.587	-15.684	1.00	117.40
	6750 6751	CB	LEU E	81 81	1.086 2.037	63.620 64.731	-16. 343 -16. 75 2	1.00 1.00	117.40 104.60
	6752	ÇG.	LEU E	81	1.348	65.795	-17.590	1.00	104.60
	6753	CD1	LEV E	81	0.269	66.455	-16.750	1.00	104.60
40	6754	CD2	LEU E	81	2.357	66.811	-18.058	1.00	104.60
	6755	Ç	LEU E	81	0.455	62.990	-17.575	1.00	117.40
	6756	0	LEU E	81	1.148	62.313	-18.325	1.00	117.40
	6757	N CA	GLU E GLU E	82	-0.844	63.186	-17.792	1.00	85.04
45	6758 6759	CB	GLU E	82 82	-1.474 -2.520	62.609 61.566	-18.982 -18.598	1.00 1.00	85.04 152.39
7,5	6760	CG	GLU E	82	-2.736	60.525	-19.684	1.00	152.39
	6761	CD	GLU E	82	-3.765	59.482	-19.297	1.00	152.39
	6762	OE1	GLU E	82	-3.785	59.083	-18.107	1.00	152.39
~~	6763	OE2	GLU E	82	-4.542	59.055	-20.185	1.00	152.39
50	6764	Ç	GLU E	82	-2.112	63.691	-19.854	1.00	85.04
	6765	0	GLU E	82	-2.843	64.562	-19.363	1.00	85.04
	6766 6767	N CA	VAL E VAL E	83 83	-1.829 -2.355	63.634 64.628	-21.152 -22.085	1.00 1.00	88.74 88.74
	6768	CB	VAL E	83	-1.258	65.146	-23.010	1.00	170.11
55	6769	CG1	VAL E	83	-1.862	66.064	-24.054	1.00	170.11
	6770	CG2	VAL E	83	-0.213	65.878	-22.197	1.00	170.11
	6771	С	VAL E	83	-3.482	64.102	-22.949	1.00	88.74
	6772	0	VAL E	83	-3.391	63.013	-23.507	1.00	88.74
60	6773		PHE E	84	-4.534	64.895	-23.091	1.00	98.95
w	6774 6775	CA CB	PHE E PHE E	84 84	-5.675 -6.017	64.451 64.273	-23.873	1.00	98.95
	6775 6776	œ	PHE E	84 84	-6.917 -6.734	63.316	-22.986 -21.864	1.00 1.00	118.45 118.45
	6777	CD1	PHE E	84	-5.997	63.674	-20.749	1.00	118.45
	6778	CD2	PHE E	84	-7.324	62.065	-21.911	1.00	118.45
65	6779	CE1	PHE E	84	-5.839	62.795	-19.701	1.00	118.45
	6780	CE2	PHE E	84	-7.172	61.173	-20.865	1.00	118.45
	6781	cz	PHE E	84	-6.434	61.541	-19.756	1.00	118.45
	6782	C	PHE E	84 84	-6.114 5.706	65.318	-25.034	1.00	· 98.95
70	6783 6784	O N	PHE E SER E	84 85	-5.736 -6.967	66.484 64.697	-25.178 -25.837	1.00 1.00	98.95
, 0	U/ 0 -7	. •	JUN L	-	-0.807	U-1.031	-50.001	1.00	152.83

	6785	CA	SER E	85	-7.592	65.304	-26.990	1.00	152.83
	6786	CB	SER E	85	-6.937	64.819	-28.279	1.00	197.25
	6787	og .	SER E	85	-7.565	65.403	-29.405	1.00	197.25
5	6788 6789	C	SER E SER E	85 85	-9.030	64.791	-26.914	1.00	152.83
,	6790	N	ASP E	86	-9.279 -9.962	63.598 65.685	-27.101 -26.600	1.00	152.83
	6791	CA	ASP E	86	-11.375	65.330	-26.494	1.00 1.00	101.99
	6792	CB	ASP E	86	-11.573	64.296	-25.386	1.00	101.99 136.02
	6793	CG	ASP E	86	-12.655	63.310	-25.715	1.00	136.02
10	6794	OD1	ASP E	86	-13.782	63.752	-26.031	1.00	136.02
	6795	OD2	ASP E	86	-12.375	62.0 9 5	-25.664	1.00	136.02
	6796	C O	ASP E	86	-12.199	66.594	-26.197	1.00	101.99
	6797 6798	N	ASP E TRP E	86 87	-11.646 -13.516	67.635 66.516	-25. 83 0	1.00	101.99
15	6799	CA	TRP E	87	-14.351	67.689	-26.356 -26.106	1.00 1.00	94.76 94.76
	6800	CB	TRP E	87	-15.806	67.417	-26.477	1.00	229.11
	6801	CG	TRP E	87	-16.051	67.695	-27.896	1.00	229.11
	6802	CD2	TRP E	87	-15.956	66.755	-28.964	1.00	229.11
20	6803	CE2	TRP E	87	-16.120	67.470	-30.165	1.00	229.11
20	6804 6805	CE3 CD1	TRP E	87	-15.735	65.372	-29.026	1.00	229.11
	6806	NE1	TRP E TRP E	87 87	-16.281 -16.319	68.917 68.787	-28.471 -29.837	1.00	229.11
	6807	CZ2	TRP E	87	-16.070	66.850	-31.411	1.00 1.00	229.11 229.11
	6808	CZ3	TRP E	87	-15.685	64.755	-30.265	1.00	229.11
25	6809	CH2	TRP E	87	-15.855	65.491	-31.438	1.00	229.11
	6810	Ç	TRP E	87	-14.273	68.108	-24.671	1.00	94.76
	6811	0	TRP E	87	-13.962	69.260	-24.355	1.00	94.76
	6812 6813	N CA	LEU E	88 88	-14.546	67.147	-23.802	1.00	160.64
30	6814	CB	LEU E	88	-14.527 -15.912	67.385 67.160	-22.379 -21.803	1.00 1.00	160.64
	6815	CG	LEU E	88	-16.950	68.149	-22.276	1.00	93.36 93.36
	6816	CD1	LEU E	88	-18.247	67.872	-21.532	1.00	93.36
	6817	CD2	LEU E	88	-16.456	69.560	-22.001	1.00	93.36
35	6818	C	LEU E	88	-13.553	66.490	-21.645	1.00	160.64
22	6819 6820	0 N	LEU E LEU E	88 89	-13.401	65.314	-21.968	1.00	160.64
	6821	CA	LEU E	89	-12.908 -11.961	67.057 66.321	-20. 63 5 -19. 82 8	1.00 1.00	107.53
	6822	CB	LEU E	89	-10.552	66.785	-20.131	1.00	107.53 83.31
	6823	CG	LEU E	89	-9.538	66.057	-19.267	1.00	83.31
40	6824	CD1	LEU E	89	-9.821	64.541	-19.311	1.00	83.31
	6825	CD2	LEU E	89	-8.138	66.385	-19.757	1.00	83.31
	6826 6827	C	LEU E LEU E	89 89	-12.252	66.573	-18.366	1.00	107.53
	6828	Ň	LEU E	90	-12.378 -12.366	67.718 65.510	-17.954 -17.576	1.00 1.00	107.53
45	6829	CA	LEU E	90	-12.629	65.676	-16.142	1.00	62.89 62.89
	6830	СВ	LEU E	90	-13.400	64,487	-15.588	1.00	49.26
	6831	CG	LEU E	90	-13.609	64.523	-14.077	1.00	49.26
	6832	CD1	LEU 3	90	-14.422	65.760	-13.775	1.00	49.26
50	6833 6834	CD2 C	LEU E	90	-14.308	63.261	-13.579	1.00	49.26
50	6835	ŏ	LEU E	90 90	-11.300 -10.515	65.773 64.830	-15.404	1.00	62.89
	6836	Ň	GLN E	91	-11.043	66.907	-15.410 -14.764	1.00 1.00	62.89 69.52
	6837	CA	GLN E	91	-9.785	67.083	-14.064	1.00	69.52
ے ہے	6838	CB	GLN E	91	-9.210	68.449	-14 388	1.00	103.30
55	6839	CG	GLN E	91	-8.977	68.644	-15.857	1.00	103.30
	6840	CD	GLN _	91	-8.226	69.921	-16.149	1.00	103.30
	6841 6842	OE1 NE2	GLN E GLN E	91 91	-8.750 -6.970	71.021	-15.967	1.00	103.30
	6843	C	GLN E	91	-6.979 -9.965	69.783 66.953	-16.599 -12.584	1.00 1.00	103.30 69.52
60	6844	Ö	GLN E	91	-10.984	67.372	-12.033	1.00	69.52
	6845	N	ALA E	92	-8.972	66.375	-11.925	1.00	61.94
	6846	CA	ALA E	92	-9 .070	66.223	-10.483	1.00	61.94
	6847 6848	CB	ALA E	92	-9.241	64.773	-10.125	1.00	129.56
65	6848 6849	C O	ALA E ALA E	92	-7.838 -6.716	66.792 66.663	-9.794	1.00	61.94
00	6850	Ň	SER E	92 93	-6.715 -8.045	66.663 67.437	-10.314 -9.643	1.00	61.94
	6851	CA	SER E	93	-6.930	68.004	-8.643 -7.904	1.00 1.00	82.97 82.97
	6852	CB	SER E	93	-7.388	68.550	-6.552	1.00	72.43
70	6853	ОG	SER E	93	-8.203	67.620	-5.871	1.00	72.43
70	6854	С	SER E	93	-5.965	66.855	-7.717	1.00	82.97
						•			

	6855	0	SER E	93	-4.873	66.846	-8.282	1.00	82.97
	6856 6857	N CA	ALA E ALA E	94	-6.395	65.865	-6.948	1.00	109.69
	6858	CB ·	ALA E	94 94	-5.588 -5.086	64.680 64.711	-6.683	1.00	109.69
5	6859	Č	ALA E	94	-6.468	63.455	-5.262 -6.910	1.00	145.34
	6860	Ö	ALA E	94	-7.652	63.488	-6.620	1.00 1.00	109.69 109.69
	6861	N	GLU E	95	-5.902	62.372	-7.431	1.00	77.50
	6862	CA	GLU E	95	-6.688	61.172	-7.711	1.00	77.50
10	6863	CB	GLU E	95	-6.065	60.391	-8.859	1.00	137.79
10	6864 6865	CG CD	GLU E GLU E	95 05	-5.979	61.195	-10.136	1.00	137.79
	6866	OE1	GLU E	95 95	-5.700 -5.582	60.335 60.901	-11.358 -12.468	1.00	137.79
	6867	OE2	GLU E	95	-5.607	59.094	-11.210	1.00 1.00	137.79
	6868	Ċ	GLU E	95	-6.869	60.258	-6.514	1.00	137.79 77.50
15	6869	0	GLU E	95	-7.723	59.376	-6.538	1.00	77.50
	6870	N	VAL E	96	-6.067	60.468	-5.470	1.00	83.99
	6871 6872	CA CB	VAL E VAL E	96 06	-6.148	59.673	-4.241	1.00	83.99
	6873	CG1	VAL E	96 96	-5.042 -5.384	58. 64 1 57.579	-4.191 -3.164	1.00	76.64
20	6874	CG2	VAL E	96	-4.856	58.037	-5.164 -5.568	1.00 1.00	76.64
	6875	С	VAL E	96	-6.009	60.634	-3.071	1.00	76.64 83.99
	6876	0	VAL E	96	-5.127	61.491	-3.057	1.00	83.99
	6877	N	VAL E	97	-6.863	60.475	-2.071	1.00	86.29
25	6878 6879	CA CB	VAL E VAL E	97 07	-6.880	61.409	-0.959	1.00	86.29
23	6880	CG1	VAL E	97 9 7	-8.028 -7.861	62.389 63.550	-1.152	1.00	80.14
	6881	CG2	VAL E	97	-8.102	62.821	-0.242 -2.571	1.00 1.00	80.14
	6882	C	VAL E	97	-7.073	60.838	0.440	1.00	80.14 86.29
20	6883	0	VAL E	97	-7.940	59.988	0.646	1.00	86.29
30	6884	N	MET E	98	-6.305	61.349	1.405	1.00	72.65
	6885 6886	CA CB	MET E	98	-6.430	60.922	2.799	1.00	72.65
	6887	CG	MET E	98 98	-5.268 -3.950	61.476 60.925	3.603 3.147	1.00	162.98
	6888	SD	MET E	98	-3.643	59.309	3.147 3.816	1.00 1.00	162.98 162.98
35	6889	CE	MET E	98	-3.249	59.757	5.511	1.00	162.98
	6890	Č	MET E	98	-7.747	61.457	3.359	1.00	72.65
	6891	0	MET E	98	-8.065	62.625	3.165	1.00	72.65
	6892 6893	N CA	GLU E	99	-8.515	60.612	4.042	1.00	91.21
40	6894	CB	GLU E	99 99	-9.789 -10.288	61.038 60.011	4.615 5.630	1.00 1.00	91.21
. •	6895	CG	GLU E	99	-11.780	60.081	5.888	1.00	221.21 221.21
	6896	CD	GLU E	99	-12.193	59.288	7,112	1.00	221.21
	6897	OE1	GLU E	99	-11.617	58.201	7.342	1.00	221.21
45	6898	OE2	GLU E	99	-13.102	59.747	7.836	1.00	221.21
77	6899 6900	C	GLU E GLU E	99 99	-9.575 -8.664	62.376	5.322	1.00	91.21
	6901	Ň	GLY E	100	-10.388	62.499 63.379	6.140 4.993	1.00 1.00	91.21
	6902	CA	GLY E	100	-10.248	64.679	5.632	1.00	149.52 149.52
50	6903	C	GLY E	100	-9.666	65.799	4.782	1.00	149.52
50	6904	0	GLY E	100	-9.830	66.974	5.111	1.00	149.52
	6905 6906	N CA	GLN E	101	-8.982	65.450	3.697	1.00	88.18
	6907	CB	GLN E	101 101	-8.381 -7.183	66.447 65.843	2.803	1.00	88.18
	6908	ČĠ	GLN E	101	-7.163 -6.053	65.456	2.072 2.988	1.00 1.00	168.37
55	6909	CD	GLN E	101	-5.680	66.573	3.934	1.00	168.37 168.37
	6910	OE1	GLN E	101	-6.363	66.812	4.923	1.00	168.37
	6911	NE2	GLN E	101	-4.598	67.272	3.630	1.00	168.37
	6912	C	GLN E	101	-9.334	67.070	1.767	1.00	88.18
60	6913 6914	O N	GLN E PRO E	101 102	-10.447	66.597	1.540	1.00	88.18
-	6915	CD	PRO E	102	-8.894 -7.628	68.148 68.898	1.116 1.252	1.00	90.47
	6916	CA	PRO E	102	-9.766	68.772	0.125	1.00 1.00	130.24 90.47
	6917	CB	PRO E	102	-9.195	70.179	0.022	1.00	130.24
65	6918	ÇG	PRO E	102	-7.727	69.923	0.124	1.00	130.24
O)	6919 6930	C	PRO E	102	-9.708	68.020	-1.203	1.00	90.47
	6920 6921	O N	PRO E LEU E	102 103	-8.713 -10.775	67.360	-1.510	1.00	90.47
	6922	CA	LEU E	103	-10.775	68.133 67.475	-1.988 -3.283	1.00 1.00	92.93
	6923	CB	LEV E	103	-11.638	66.186	-3.160	1.00	92,93 78.05
70	6924	CG	LEV E	103	-11.718	65.529	-4.528	1.00	78.05 78.05
						•			. 5.00

	6925 6926	CD1 CD2	LEU E	103 103	-10.330 -12.618	65.172 64.299	-4.969 -4.466	1.00 1.00	78.05 78.05
	6927	С	LEU E	103	-11.556	68.364	-4.296	1.00	92.93
-	6928	0	LEU E	103	-12.690	68.784	-4.071	1.00	92.93
5	6929	N	PHE E	104	-10.906	68.654	-5.413	1.00	62.11
	6930	CA	PHE E	104	-11.557	69.491	-6.406	1.00	62.11
	6931	CB	PHE E	104	-10.792	70.814	-6.607	1.00	152.14
	6932	CG	PHE E	104	-10.639	71.636	-5.354	1.00	152.14
	6933	CD1	PHE E	104	-9.688	71.298	-4.401	1.00	152.14
10	6934	CD2	PHE E	104	-11.439	72.760	-5.132	1.00	152.14
	6935	CE1	PHE E	104	-9.537	72.054	-3.235	1.00	152.14
	6936	CE2	PHE E	104	-11.297	73.526	-3.967	1.00	152.14
	6937	CZ	PHE E	104	-10.338	73.173	-3.020	1.00	152.14
	6938	С	PHE E	104	-11.672	68.775	-7.759	1.00	62.11
15	6939	0	PHE E	104	-10.686	68.246	-8.269	1.00	62.11
	6940	N	LEU E	105	-12.871	68.748	-8.336	1.00	83.91
	6941	CA	LEU E	105	-13.074	68.140	-9.651	1.00	83.91
	6942	CB	LEU E	105	-14.208	67.119	-9.618	1.00	47.95
-	6943	CG	LEU E	105	-14.010	66.057	-8.551	1.00	47.95
20	6944	CD1	LEU E	105	-15.076	64.958	-8.677	1.00	47.95
	6945	CD2	LEU E	105	-12. 63 3	65.508	-8.729	1.00	47.95
	6946	С	· LEU E	105	-13.454	69.279	-10.565	1.00	83.91
	6947	0	LEU E	105	-14.110	70.224	-10.133	1.00	83.91
0.5	6948	N '	ARG E	106	-13.063	69.201	-11.824	1.00	105.55
25	6949	CA	ARG E	106	-13.391	70.273	-12.737	1.00	105.55
	6950	CB	ARG E	106	-12,132	71.181	-12.874	1.00	149.26
	6951	CG	ARG E	106	-12.358	72.290	-13.865	1.00	149.26
	6952	CD	ARG E	106	-11.036	72.987	-14.126	1.00	149.26
20	6953	NE	ARG E	106	-11.165	74.010	-15.158	1.00	149.26
30	6954	CZ	ARG E	106	-10.153	74.477	-15.880	1.00	149.26
	6955	NH1	ARG E	106	-8.925	74.013	-15.691	1.00	149.26
	6956	NH2	ARG E	106	-10.374	75.404	-16.800	1.00	149.26
	6957	C	ARG E	106	-13.804	69.761	-14.110	1.00	105.55
25	6958	0	ARG E	106	-13.044	69.027	-14.734	1.00	105.55
35	6959	N	CYS E	107	-15.000	70.118	-14.585	1.00	115.02
	6960	CA	CYS E	107	-15.400	69.665	-15.913	1.00	115.02
	6961	Č	CYS E	107	-14.789	70.673	-16.856	1.00	115.02
	6962	0	CYS E	107	-15.230	71.813	-16.932	1.00	115.02
40	6963	CB	CYS E	107	-16.914	69.630	-16.079	1.00	134.10
40	6964	SG	CYS E	107	-17.441	68.605	-17.498	1.00	134.10
	6965	N	HIS E	108	-13.755	70.242	-17.562	1.00	96.54
	6966	CA	HIS E	108	-13.017	71.109	-18.460	1.00	96.54
	6967	CB	HIS E	108	-11.535	70.876	-18.240	1.00	124.72
45	6968	CG	HIS E	108	-10.657	71.846	-18.959	1.00	124.72
43	6969	CD2	HIS E	108	-9.644	71.651	-19.836	1.00	124.72
	6970	ND1	HIS E	108	-10.737	73.207	-18.759	1.00	124.72
	6971	CE1	HIS E	108	-9.806	73.807	-19.480	1.00	124.72
	6972	NE2	HIS E	108	-9.128	72.886	-20.142	1.00	124.72
50	6973 6974	C	HIS E	108	-13. 328	70.954	-19.938	1.00	96.54
50	6975	0	HIS E	108	-13.224	69.864	-20.506	1.00	98.54
	6976	N	GLY E	109	-13.680	72.070	-20.563	1.00	176.91
		CA	GLY E	109	-13.999	72.050	-21.973	1.00	177.91
	6977 6978	C	GLY E	109	-12.753	72.194	-22.815	1.00	176.91
55		0	GLY E	109	-11.737	72.706	-22.349	1.00	176.91
55	6979 6980	N	TRP E	110	-12.826	71.732	-24.056	1.00	146.96
	6981	CA	TRP E	110	-11.696	71.836	-24.956	1.00	146.96
	6982	CB	TRP E	110	-11.982	71.061	-26.241	1.00	177.84
	6983	CG	TRP E	110	-10.936	71.248	-27.286	1.00	177.84
60	6984	CD2 CE2	TRP E	110	-9.797	70.415	-27.514	1.00	177.84
00	6985	CE3	TRP E	110	-9.056	70.996	-28.564	1.00	177.84
	6986		TRP E	110	-9.331	69.226	-26.932	1.00	177.84
	6987	CD1	TRP E	110	-10.845	72.273	-28.180	1.00	177.84
	6988	NE1	TRP E	110	-9.718	72.131	-28.953	1.00	177.84
65		CZ2	TRP E	110	-7.875	70.433	-29.047	1.00	177.84
05	6989	CZ3	TRP E	110	-8.153	68.667	-27.413	1.00	177.84
	6990	CH2	TRP E	110	-7.439	69.273	-28.459	1.00	177.84
	6991	C	TRP E	110	-11.404	73.303	-25.275	1.00	146.96
	6992 6993	0	TRP E	110	-12.300	74.154	-25.255	1.00	146.96
70	6994	N	ARG E	111	-10.136	73.594	-25.551	1.00	199.97
, 0	V44	CA	ARG E	111	-9.716	74.948	-25.887	1.00	199.97

	6995	СВ	ARG E	111	-10.136	75.282	-27.295	1.00	249.42
	6996	CG	ARG E	111	-9.116	74.871	-28.285	1.00	249.42 249.42
	6997	CD.	ARG E	111	-9.462	75.454	-29.595	1.00	249.42
5	6998 6999	NE .	ARG E	111	-8.270	75.956	-30.249	1.00	249.42
,	7000	CZ NH1	ARG E ARG E	111	-7.559	76.996	-29.814	1.00	249.42
	7001	NH2	ARG E	111 111	-7.918 -6.472	77.656 77.367	-28.711	1.00	249.42
	7002	Ċ	ARG E	111	-10.262	76.009	-30.483	1.00	249.42
	7003	Ō	ARG E	111	-10.388	77.173	-24.972 -25.350	1.00	199.97
10	7004	N	ASN E	112	-10.597	75.590	-23.767	1.00 1.00	199.97
	7005	CA	ASN E	112	-11.129	76.482	-22.769	1.00	112.19 112.19
	7006	CB	ASN E	112	-10.101	77.553	-22.432	1.00	133.79
	7007	CG	ASN E	112	-10.330	78.144	-21.061	1.00	133.79
15	7008 7009	OD1 ND2	ASN E ASN E	112	-11.446	78.097	-20.531	1.00	133.79
13	7010	C	ASN E ASN E	112 112	-9.280	78.710	-20.478	1.00	133.79
	7011	ŏ	ASN E	112	-12.445 -12.776	77.147	-23.163	1.00	112.19
	7012	Ň	TRP E	113	-13.200	78.218 76.532	-22.651	1.00	112.19
	7013	CA	TRP E	113	-14.478	77.116	-24.067 -24.441	1.00	154.00
20	7014	CB	TRP E	113	-15.153	76.326	-25.542	1.00 1.00	154.00
	7015	CG	TRP E	113	-14.586	76.595	-26.860	1.00	235.27 235.27
	7016	CD2	TRP E	113	-14.400	75.651	-27.909	1.00	235.27
	7017	CE2	TRP E	113	-13.885	76.353	-29.018	1.00	235.27
25	7018	CE3	TRP E	113	-14.628	74.270	-28.027	1.00	235.27
45	7019 7020	CD1	TRP E	113	-14.180	77.804	-27.348	1.00	235.27
	7020 7021	NE1 CZ2	TRP E	113	-13.758	77.667	-28.647	1.00	235.27
	7022	CZ3	TRP E	113 113	-13.592	75.726	-30.229	1.00	235.27
	7023	CH2	TRP E	113	-14.335 -13.818	73.643	-29.233	1.00	235.27
30	7024	Ċ _	TRP E	113	-15.400	74.373 77.133	-30.318 -23.246	1.00	235.27
	7025	Ö	TRP E	113	-14.983	76.886	-23.246 -22.116	1.00 1.00	154.00
	7026	N	ASP E	114	-16.664	77.430	-23.503	1.00	154.00 242.58
	7027	CA	ASP E	114	-17.649	77.470	-22.442	1.00	242.58
25	7028	CB	ASP E	114	-18.418	78.794	-22.471	1.00	249.32
35	7029	CG	ASP E	114	-17.656	79.922	-21.803	1.00	249.32
	7030 7031	OD1 OD2	ASP E	114	-17.348	79.791	-20.599	1.00	249.32
	7031	C	ASP E ASP E	114	-17.365	80.933	-22.475	1.00	249.32
	7033	ŏ	ASP E	114 114	-18.606 -19.027	76.306 75.942	-22.572	1.00	242.58
40	7034	Ň	VAL E	115	-18.931	75. 84 2 75.717	-23.672 -21.430	1.00	242.58
	7035	CA	VAL E	115	-19.846	74.594	-21.430	1.00 1.00	148.92
	7036	CB	VAL E	115	-19.199	73.377	-20.746	1.00	148.92 243.92
	7037	CG1	VAL E	115	-20.086	72.162	-20.949	1.00	243.92
45	7038	CG2	VAL E	115	-17.821	73.161	-21.331	1.00	243.92
43	7039 7040	C	VAL E	115	-21.075	74.959	-20.581	1.00	148.92
•	7040	0 N	VAL E TYR E	115	-20.985	75.672	-19.577	1.00	148.92
	7042	CA	TYR E	116 116	-22.226	74.466	-21.020	1.00	86.50
	7043	CB	TYR E	116	-23.470 -24.374	74.752 75.633	-20.320	1.00	86.50
50	7044	ČĞ	TYR E	116	23.782	76.991	-21.192 -21.517	1.00	249.77
	7045	CD1	TYR E	116	-23.088	77.210	-22.709	1.00 1.00	249.77
	7046	CE1	TYR E	116	-22.513	78.454	-22.994	1.00	249.77 249.77
	7047	CD2	TYR E	116	-23.889	78.048	-20.616	1.00	249.77
55	7048	CE2	TYR E	116	-23.319	79.293	-20.886	1.00	249.77
55	7049	CZ	TYR E	116	-22.631	79.488	-22.075	1.00	249.77
	7050 7051	он	TYR E	116	-22.051	80.710	-22.336	1.00	249.77
	7052	C	TYR E TYR E	116	-24.208	73.466	-19.940	1.00	86.50
	7053	Ň	LYS E	116 117	-23.829	72.356	-20.362	1.00	86.50
60	7054	ČA	LYS E	117	-25.277 -26.078	73.630 72.500	-19.164	1.00	217.77
	7055	CB	LYS E	117	-26.963	71.967	-18.707 -19.832	1.00	217.77
	7056	CG	LYS E	117	-28.295	72.674	-19.832 -19.997	1.00 1.00	191.92
	7057	CD	LYS E	117	-29.246	71.813	-20.819	1.00	191.92
<i>C</i> =	7058	CE	LYS E	117	-29.481	70.462	-20.143	1.00	191.92 191.92
65	7059	NZ	LYS E	117	-30.376	69.560	-20.915	1.00	191.92
	7060	C	LYS E	117	-25.161	71.387	-18.230	1.00	217.77
	7061 7062	0 N	LYS E	117	-25.228	70.262	-18.724	1.00	217.77
	7062 7063	CA	VAL E VAL E	118	-24.306	71.709	-17.268	1.00	181.28
70	7064	CB	VAL E	118 118	-23.356 -22.089	70.743	-16.731	1.00	181.28
	•		*/% E	110	-EE.V08	71.444	-16.254	1.00	157.61

	7065	CG1	VAL E	118	-21.427	70.628	45 474	4.00	
	7066	CG2	VAL E	118	-21.141	70.628 71.619	-15.171 -17.420	1.00 1.00	157.61
	7067	Ç.	VAL E	118	-23.857	69.864	-15.598	1.00	157.61 181.28
5	7068 7069	O N	VAL E	118	-24.500	70.335	-14.661	1.00	181.28
,	7070	CA	ILE E	119 119	-23.514 -23.932	68.585 67.630	-15.674	1.00	95.37
	7071	CB	ILE E	119	-25.932 -25.093	67.630 66.783	-14.665 -15.1 8 4	1.00	95.37
	7072	CG2	ILE E	119	-25.598	65.858	-14.102	1.00 1.00	80.86
10	7073	CG1	ILE E	119	-26.198	67.695	-15.696	1.00	80.86 80.86
10	7074 7075	CD1	ILE E	119	-27.227	66.956	-16.527	1.00	80.86
	7075 7076	C	ILE E ILE E	119	-22.791	66.678	-14.348	1.00	95.37
	7077	Ň	TYR E	119 120	-22.280 -22.373	66.017 66.602	-15.249	1.00	95.37
	7078	CA	TYR E	120	-21.315	65.664	13.088 -12.732	1.00 1.00	103.71
15	7079	CB	TYR E	120	-20.499	66.128	-11.550	1.00	103.71 87.63
	7080	CG	TYR E	120	-19.634	67.303	-11.821	1.00	87.63
	7081 7082	CD1 CE1	TYR E	120	-20.141	68.575	-11.746	1.00	87.63
	7083	CD2	TYR E TYR E	120 120	-19.351 -18.300	69.666 67.141	-12.010	1.00	87.63
20	7084	CE2	TYR E	120	-17.486	67.141 68.226	-12.171 -12.447	1.00	87.63
	7085	CZ	TYR E	120	-18.017	69.490	-12.366	1.00 1.00	87.63
	7086	ŌН	TYR E	120	-17.220	70.579	-12.651	1.00	87.63 87.63
	7087	C	TYR E	120	-21.972	64.380	-12.305	1.00	103.71
25	7088 7089	0 N	TYR E	120	-23.037	24.401	-11.694	1.00	103.71
20	7090	CA	TYR E TYR E	121 121	-21.324	63.263	-12.596	1.00	62.69
	7091	CB	TYR E	121	-21.857 -22.202	61.963 61.148	-12.221	1.00	62.69
	7092	CG	TYR E	121	-23.364	61.653	-13.476 -14.309	1.00 1.00	95.66
20	7093	CD1	TYR E	121	-23.288	62.865	-14.992	1.00	95.66 95.66
30	7094	CE1	TYR E	121	-24.334	63.305	-15.806	1.00	95.66
	7095 7096	CD2 CE2	TYR E TYR E	121	-24.522	60.885	-14.455	1.00	95.66
	7097	CZ	TYR E	· 121	-25.576	61.315	-15.269	1.00	95.66
	7098	OH	TYR E	121	-25.477 -26.515	62.527 62.943	-15.945 -16.761	1.00	95.66
35	7099	С	TYR E	121	-20.873	61.165	-11.368	1.00 1.00	95.66 62.60
	7100	0	TYR E	121	-19.667	61.179	-11.620	1.00	62.69 62.69
	7101	N	LYS E	122	-21.391	60.478	-10.356	1.00	76.05
	7102 7103	CA CB	LYS E Lys e	122	-20.562	59.633	-9.521	1.00	76.05
40	7104	CG	LYS E	122 122	-20.410 -19.516	60.198	-8.114	1.00	107.43
	7105	CD	LYS E	122	-19.635	59.339 59.698	-7.238 -5.779	1.00 1.00	107.43
	7106	CE	LYS E	122	-18.887	58.706	-4.914	1.00	107.43 107.43
	7107	NZ	LYS E	122	-19.161	58.998	-3.484	1.00	107.43
45	7108 7109	CO	LYS E	122	-21.223	58.263	-9.440	1.00	76.05
73	7110	N	LYS E ASP E	122 123	-22.325 -20.543	58.127	-8.898	1.00	76.05
	7111	CA	ASP E	123	-20.543 -21.059	57.252 55.892	-9.973	1.00	138.97
	7112	СВ	ASP E	123	-21.188	55.363	-9.976 -8.545	1.00 1.00	138.97
50	7113	CG	ASP E	123	-19.849	54.991	-7.945	1.00	185.30 185.30
50	7114 7115	OD1	ASP E	123	-19.068	54.303	-8.638	1.00	185.30
	7116	OD2 C	ASP E ASP E	123	-19.578	55.374	-6.785	1.00	185.30
	7117	ŏ	ASP E	123 123	-22.396 -23.333	55.792 55.147	-10.702	1.00	138.97
	7118	Ň	GLY E	124	-22.472	55.147 56.443	-10.225 -11.862	1.00	138.97
55	7119	CA	GLY E	124	-23.675	56.412	-12.675	1.00 1.00	163,35 163,35
	7120	Ç	GLY E	124	-24.838	57.262	-12.200	1.00	163.35
	7121	0	GLY E	124	-25.840	57.388	-12.907	1.00	163.35
	7122 7123	N CA	GLU E	125	-24.711	57.854	-11.016	1.00	131.17
60	7124	CB	GLU E	125 125	-25.777 -25.822	58.684 58.535	-10.447	1.00	131.17
	7125	ČĠ	GLU E	125	-26.269	57.168	-8.911 -8.368	1.00	143.41
	7126	CD	GLU E	125	-27.780	56.971	-8.384	1.00 1.00	143.41 143.41
	7127	OE1	GLU E	125	-28.492	57.744	-7.700	1.00	143.41
65	7128	OE2	GLU E	125	-28.249	56.040	-9.077	1.00	143.41
	7129 7130	C	GLU E	125	-25.597	60.160	-10.771	1.00	131.17
	7131	Ň	ALA E	125 126	-24.483 -26.695	60.656	-10.809	1.00	131.17
	7132	ĊA	ALA E	126	-26.604	60.864 62.290	-11.006	1.00	115.32
70	7133	СВ	ALA E	126	-27.979	62.844	-11.265 -11.605	1.00 1.00	115.32 168.61
70	7134	С	ALA E	126	-26.104	62.855	-9.935	1.00	115.32
						•			

	7135	0	ALA E	126	-26.467	62.339	-8.876	1.00	115.32
	7136	N	LEU E	127	-25.275	63.897	-9.967	1.00	118.41
	7137	CA.	LEU E	127	-24.752	64.458	-8.714	1.00	118.41
5	7138 7139	CB	LEU E	127	-23.271	64.162	-8.577	1.00	111.80
,	7140	CD1	LEV E	127 127	-22.934	64.190	-7.090	1.00	111.80
	7141	CD2	LEU E	127	-23.811 -21.465	63.158 63.889	-6.384 6.900	1.00	111.80
	7142	C	LEU E	127	-24.957	65.947	-6.868 -8.453	1.00	111.80
	7143	Ō	LEU E	127	-25.470	66.328	-7.404	1.00 1.00	118.41
10	7144	N	LYS E	128	-24.498	66.785	-9.373	1.00	118.41 133.41
	7145	CA	LYS E	128	-24.677	68.228	-9.259	1.00	133.41
	7146	СВ	LYS E	128	-23.405	68.893	-8.760	1.00	171.72
	7147	CG	LYS E	128	-22.965	68.445	-7.388	1.00	171.72
15	7148 7149	CD CE	LYS E	128	-23.865	68.977	-6.284	1.00	171.72
13	7150	NZ	LYS E LYS E	128 128	-23.287 -24.024	68.616	-4.917	1.00	171.72
	7151	C	LYS E	128	-25.015	69.227 68.757	-3.779	1.00	171.72
	7152	ŏ	LYS E	128	-24.626	68.153	-10.653 -11.657	1.00	133.41
	7153	Ň	TYR E	129	-25.733	69.87	-10.729	1.00 1.00	133.41
20	7154	CA	TYR E	129	-26.106	70.442	-12.029	1.00	159.58 159.58
	7155	CB	TYR E	129	-27.496	69.983	-12.438	1.00	246.12
	7156	CG	TYR E	129	-28.122	70.887	-13.441	1.00	246.12
	7157	CD1	TYR E	129	-27.756	70.809	-14.781	1.00	246.12
25	7158	CE1	TYR E	129	-28.298	71.675	-15.715	1.00	246.12
25	7159	CD2	TYR E	129	-29.063	71.857	-13.055	1.00	246.12
	7160 7161	CE2 CZ	TYR E	129	-29.624	72.721	-13.990	1.00	246.12
	7162	OH	TYR E TYR E	129 129	-29.236 -29.822	72.624	-15.326	1.00	246.12
	7163	č.	TYR E	129	-26.106	73.442 71.953 .	-16.274	1.00	246.12
30	7164	ŏ	TYRE	129	-26.579	71.933 . 72.589	-12.048 -11.112	1.00	159.58
	7165	N	TRP E	130	-25.600	72.526	-13.137	1.00 1.00	159.58
	7166	CA	TRP E	130	-25.557	73.976	-13.280	1.00	184.49 184.49
	7167	СВ	TRP E	130	-24.211	74.535	-12.817	1.00	245.42
25	7168	CG	TRP E	130	-23.751	74.067	-11.472	1.00	245.42
35	7169	CD2	TRP E	130	-23.750	74.828	-10.257	1.00	245.42
	7170 7171	CE2 CE3	TRP E	130	-23.186	74.005	-9.254	1.00	245.42
	7172	CD1	TRP E	130	-24.179	76.119	-9.918	1.00	245.42
	7173	NE1	TRP E	130 130	-23.202 -22.859	72.856	-11.166	1.00	245.42
40	7174	CZ2	TRPE	130	-23.034	72.811 74.438	-9.835 -7.930	1.00	245.42
	7175	CZ3	TRP E	130	-24.028	76.548	-8.600	1.00 1.00	245.42
	7176	CH2	TRP E	130	-23.454	75.709	-7.626	1.00	245.42 245.42
	7177	С	TRP E	130	-25.768	74.407	-14.725	1.00	184.49
45	7178	0 '	TRP E	130	-25.711	73.584	-15.638	1.00	184.49
43	7179	N	TYR E	131	-26.014	75.701	-14.930	1.00	185.41
	7180 7181	CA CB	TYR E	131	-26.187	76.228	-16 <i>.2</i> 77	1.00	185.41
	7182	CG	TYR E TYR E	131	-27.063	77.477	-16.282	1.00	249.42
	7183	CD1	TYR E	131 131	-27.438 -28.391	77.858 77.125	-17.685	1.00	249.42
50	7184	CE1	TYRE	131	-28.654	77.384	-18.389 -19.728	1.00	249.42
	7185	CD2	TYR E	131	-26.755	78.869	-18.358	1.00 1.00	249.42
	7186	CE2	TYR E	131	-26.997	79.127	-19.703	1.00	249.42 249.42
	7187	CZ	TYR E	131	-27.951	78.384	-20.380	1.00	249.42 249.42
55	7188	ÓН	TYR E	131	-28.189	78.642	-21.710	1.00	249.42
<i>JJ</i>	7189	C	TYR E	131	-24.780	76.577	-16.758	1.00	185.41
	7190 7191	0 N	TYTE	131	-24.141	<u>75.784</u>	-17.455	1.00	185.41
	7192	CA CA	GLU E	132 132	-24.310	77.777	-16.415	1.00	229.70
	7193	CB	GLU E	132	-22.942 -22.638	78.159	-16.751	1.00	229.70
60	7194	CG	GLU E	132	-23.207	79.608 80.700	-16.344	1.00	249.20
	7195	CD	GLU E	132	-22.123	81.565	-17 <i>.2</i> 58 -17.898	1.00	249.20
	7196	OE1	GLU E	132	-20.982	81.562	-17.392	1.00 1.00	249.20
	7197	OE2	GLU E	132	-22.412	82.255	-18.899	1.00	249.20 249.20
6 6	7198	Ç	GLU E	132	-22.290	77.200	-15.773	1.00	249.20
65	7199	0	GLU E	132	-22.652	77.190	-14.595	1.00	229.70
	7200	N	ASN E	133	-21.348	76.385	-16.233	1.00	219.94
	7201 7202	CA	ASN E	133	-20.764	75.401	-15.332	1.00	219.94
	7202 7203	CB CG	ASN E	133	-19.878	74.415	-16.095	1.00	129.08
70	7203 7204	OD1	ASN E ASN E	133 133	-18.469	74.898	-16.252	1.00	129.08
		U	WHITE	100	-18.235	76.020	-16.692	1.00	129.08

	7205	ND2	ACM E	400	47 540				
	7205 7206	C NU2	ASN E ASN E	133	-17.510	74.046	-15.904	1.00	129.08
	7207	ŏ	ASN E	133	-20.023	75.919	-14.118	1.00	219.94
	7208	Ň.	HIS E	133 134	-19.802	77.115	-13.944	1.00	219.94
5	7209	ČA	HIS E	134	-19.638 -18.970	74.965 75.231	-13.286	1.00	192.14
•	7210	ČB	HIS E	134	-20.007	75.231 75.079	-12.036	1.00	192.14
	7211	ČĞ	HIS E	134	-19.514	75.463	-10.924	1.00	214.14
	7212	CD2	HIS E	134	-19.356	74.731	-9.567 -8.436	1.00	214.14
	7213	ND1	HIS E	134	-19.138	76.749	-9.245	1.00	214.14
10	7214	CE1	HIS E	134	-18.771	76.794	-7.976	1.00	214.14
	7215	NE2	HIS E	134	-18.895	75.584	•7.463	1.00 1.00	214.14
	7216	С	HIS E	134	-17.828	74.231	-11.860	1.00	214.14
	7217	0	HIS E	134	-17.412	73.574	-12.820	1.00	192.14
	7218	N	ASN E	135	-17.336	74.114	-10.630	1.00	192.14
15	7219	CA	ASN E	135	-16.246	73.208	-10.311	1.00	109.49 109.49
	7220	CB	ASN E	135	-14.921	73.967	-10.346	1.00	216.32
	7221	CG	ASN E	135	-14.571	74.433	-11.741	1.00	216.32
	7222	OD1	ASN E	135	-14.694	73.661	-12.691	1.00	216.32
00	7223	ND2	ASN E	135	-14.125	75.677	-11.883	1.00	216.32
20	7224	С	ASN E	135	-16.462	72.573	-8.957	1.00	109.49
	7225	0	ASN E	135	-15.9 6 0	73.058	-7.948	1.00	109.49
	7226	N.	ILE E	136	-17.223	71.484	-8.949	1.00	98.56
	7227	. CA	ILE E	136	-17.541	70.753	-7.725	1.00	98.56
25	7228	CB	ILE E	136	-18.026	69.322	· -8.063	1.00	164.42
25	7229	CG2	ILE E	136	-17.070	68.654	-9.020	1.00	164.42
	7230	CG1	ILE E	136	-18.182	68.505	-6.792	1.00	164.42
	7231	CD1	ILE E	136	-18.771	67.146	-7.055	1.00	164.42
	7232	Ç	ILE E	136	-16.351	70.717	-6.779	1.00	98.56
30	7233	0	ILE E	136	-15.300	70.168	-7.104	1.00	98.56
30	7234	N OA	SER E	137	-16.524	71.329	-5.613	1.00	114.80
	7235 7236	CA CB	SER E	137	-15.462	71.405	-4.622	1.00	114.80
	7236 7237	OG	SER E	137	-15.128	72.866	-4.360	1.00	96.11
	7238	C	SER E	137	-14.336	72.997	-3.196	1.00	96.11
35	7239	ŏ	SER E SER E	137	-15.798	70.714	-3.303	1.00	114.80
-	7240	Ň	ILE E	137 138	-16.955	70.690	-2.879	1.00	114.80
	7241	ČA	ILE E	138	-14.773	70.169	-2.652	1.00	105.32
	7242	CB	ILE E	138	-14. 93 9 -14.851	69.466 67.060	-1.382	1.00	105.32
	7243	CG2	ILE E	138	-14.767	67.969 67.296	-1.577	1.00	81.88
40	7244	CG1	ILE E	138	-16.049	67.484	-0.223 -2.408	1.00	81.88
	7245	CD1	ILE E	138	-15.917	66.048	-2.408 -2.912	1.00	81.88
	7246	С	ILE E	138	-13.869	69.833	-0.374	1.00 1.00	81.88
	7247	0	ILE E	138	-12.686	69.614	-0.619	1.00	105.32 105.32
	7248	N	THR E	139	-14.283	70.362	0.772	1.00	128.39
45	7249	CA	THR E	139	-13.333	70.758	1.807	1.00	128.39
	7250	СВ	THR E	139	-13.986	71.743	2.788	1.00	173.5-
	7251	OG1	THR E	139	-15.220	71.194	3.265	1.00	173.94
	7252	CG2	THR E	139	-14.267	73.071	2.094	1.00	173.94
50	7253	Ç	THR E	139	-12.825	69.535	2.566	1.00	128.39
50	7254	0	THR E	139	-11.709	69.058	2.337	1.00	128.39
	7255	N _.	ASN E	140	-13.650	69.041	3.480	1.00	224.25
	7256	CA	ASN E	140	-13.323	67.859	4.263	1.00	224.25
	7257	CB	ASN E	140	-14.012	67.918	5.625	1.00	231.48
55	7258	CG	ASN E	140	-13.813	66.656	6.429	1.00	231.48
22	7239	OD1	ASN E	140	-13.998	65.547	5.923	1.00	231.43
	7260 7261	ND2	ASN E	140	-13.443	66.823	7.692	1.00	231.40
		Ç	ASN E	140	-13.874	66.691	3.464	1.00	224.25
	7262 7263	0	ASN E	140	-15.073	66.629	3.204	1.00	224.25
60	7264	N CA	ALÁ E	141	-13.004	65.763	3.086	1.00	132.13
00	7265	CB	ALA E	141	-13.420	64.623	2.289	1.00	132.13
	7266	C	ALA E ALA E	141	-12.374	64.323	1.257	1.00	95.25
	7267	ŏ		141	-13.730	63.367	3.072	1.00	132.13
	7268	N	ALA E THR E	141	-12.932	62.901	3.884	1.00	132.13
65	7269	CA	THR E	142	-14.903	62.811	2.802	1.00	103.70
	7270	CB	THR E	142 142	-15.339	61.588	3.454	1.00	103.70
	7271	OG1	THR E	142	-16.873	61.526	3.477	1.00	152.79
	7272	CG2	THR E	142	-17.384 -17.346	62.747 60.276	4.028	1.00	152.79
	7273	Č	THR E	142	-17.346	60.376 60.417	4.329	1.00	152.79
70	7274	ō	THR E	142	-14.198	60.624	2.650 1.575	1.00	103.70
				. 12	17.100	00.024	1.575	1.00	103.70

	7275 7276	N CA	VAL E	143 143	-14.887 -14.369	59.197 58.042	3.164 2.437	1.00 1.00	124.54 124.54
	7277	CB.	VAL E	143	-14.026	56.863	3.365	1.00	132.81
5	7278	CGf	VAL E	143	-15.292	56.315	3.999	1.00	132.81
3	7279	CG2	VAL E	143	-13.310	55.773	2.577	1.00	132.81
	7280 7281	C	VAL E	143	-15.448	57.583	1.484	1.00	124.54
	7281 7282	N	VAL E GLU E	143	-15.187	56.822	0.555	1.00	124.54
	7283	CA	GLU E	144 144	-16.668 -17.781	58.047 57.678	1.722	1.00	123.03
10	7284	CB	GLU E	144	-19.108	57.964	0.863 1.558	1.00	123.03
	7285	ČĞ	GLU E	144	-19.323	57.136	2.812	1.00 1.00	249.45
	7286	CD	GLU E	144	-19.316	57.978	4.073	1.00	249.45 249.45
	7287	OE1	GLU E	144	-20.163	58.892	4.176	1.00	249.45
	7288	OE2	GLU E	144	-18.470	57.730	4.958	1.00	249.45
15	7289	Ç	GLU E	144	-17.709	58.428	-0.460	1.00	123.03
	7290	0	GLU E	144	-18.373	58.051	-1.416	1.00	123.03
	7291	N.	ASP E	145	-16.897	59.485	-0.509	1.00	78.25
	7292 7293	CA	ASP E	145	-16.721	60.284	-1.726	1.00	78.25
20	7293 7294	CB CG	ASP E ASP E	145 145	-16.017	61.593	-1.396	1.00	126.03
20	7295	OD1	ASP E	145	-16.912 -17.955	62.551 62.900	-0.679	1.00	126.03
	7296	OD2	ASP E	145	-16.581	62.944	-1.272 0.465	1.00 1.00	126.03
	7297	Č	ASP E	145	-15.918	59.528	-2.789	1.00	126.03 78.25
	7298	Ó	ASP E	145	-15.889	59.920	-3.952	1.00	78.25
25	7299	N	SER E	146	-15.263	58.442	-2.388	1.00	91.78
	7300	CA	SER E	146	-14.482	57.660	-3.331	1.00	91.78
	7301	СВ	SER E	146	-13.708	56.568	-2.591	1.00	200.20
	7302	OG	SER E	146	-12.805	57.145	-1.661	1.00	200.20
30	7303	C	SER E	146	-15.448	57.065	-4.335	1.00	91.78
30	7304 7305	0 N	SER E	146	-16.558	56.675	-3.981	1.00	91.78
	7306	CA	GLY E GLY E	147 147	-15.039	57.020	-5.592	1.00	97.94
	7307	Č	GLY E	147	-15.910 -15.365	56.484 56.777	-6.622 -8.007	1.00	97.94
	7308	ŏ	GLY E	147	-14.177	57.079	-8.007 -8.146	1.00 1.00	97.94
35	7309	Ň	THR E	148	-16.211	56.677	-9.033	1.00	97.94 66.84
	7310	CA	THR E	148	-15.767	56.955	-10.399	1.00	66.84
	7311	СВ	THR E	148	-15.794	55.674	-11.285	1.00	76.59
	7312	OG1	THR E	148	-16.932	55.699	-12.141	1.00	76.59
40	7313	CG2	THR E	148	-15.880	54.450	-10.424	1.00	76.59
40	7314 7315	CO	THR E THR E	148	-16.662	58.055	-10.978	1.00	66.84
	7316	Ň	TYR E	148 149	-17.884 -16.041	57.889 50.487	-11.145	1.00	66.84
	7317	CA	TYR E	149	-16.768	59.187 60.335	-11.273 -11.774	1.00	55.84
	7318	CB	TYR E	149	-16.262	61.585	-11.070	1.00 1.00	55.84 63.87
45	7319	CG	TYR E	149	-16.445	61.611	-9. 57 5	1.00	63.87
	7320	CD1	TYR E	149	-15.728	60.766	-8.730	1.00	63.87
	7321	CE1	TYR E	149	-15.895	60.837	-7.342	1.00	63.87
	7322	CD2	TYR E	149	-17.326	62.515	-9.003	1.00	63.87
50	7323	CE2	TYR E	149	-17.502	62.597	-7.63 9	1.00	63.87
30	7324	CZ	TYR E	149	-16.793	61.761	-6.812	1.00	63.87
	7325 7326	OH C	TYR E	149	-17.022	61.871	-5.455	1.00	63.87
	7327	ŏ	TYR E TYR E	149	-16.630 -15.790	60.541	-13.274	1.00	55.84
	7328	Ň	TYR E	149 150	-15.789 -17.478	59.909 61.414	-13.918	1.00	55.84
55	7329	CA	TYR E	150	-17.463	61.805	-13.817 -15.227	1.00 1.00	90.25
	7330	СВ	TYR E	150	-17.811	60.622	-16.175	1.00	90.25 141.76
	7331	CG	TYR E	150	-19.266	60.196	-16.334	1.00	141.76
	7332	CD1	TYR E	150	-20.183	60.995	-17.006	1.00	141.76
60	7333	CE1	TYR E	150	-21.503	60.584	-17.180	1.00	141.76
60	7334	CD2	TYR E	150	-19.711	58.965	-15.839	1.00	141.76
	7335	CE2	TYR E	150	-21.030	58.545	-16.010	1.00	141.76
	7336 7337	CZ	TYR E	150	-21.924	59.359	-16.678	1.00	141.76
	7337 7338	OH C	TYR E	150	-23.239	58.958	-16.823	1.00	141.76
65	7339	ŏ	TYR E TYR E	150 150	-18.481 -19.308	62.934 63.056	-15.293	1.00	90.25
	7340	Ň	CYS E	151	-18.404	63.792	-14.388 -16.309	1.00	90.25
	7341	ĈA	CYS E	151	-19.360	64.895	-16.421	1.00 1.00	89.54 89.54
	7342	C	CYS E	151	-19.945	65.031	-17.811	1.00	89.54
70	7343	0	CYS E	151	-19.354	64.573	-18.778	1.00	89.54
70	7344	CB	CYS E	151	-18.713	66.218	-16.017	1.00	116.04

	7045	00	ov.o =						
	7345 7346	SG N	CYS E		-17.189	66.664	-16.901	1.00	116.04
	7347	ČA	THR E		-21.118	65.650 65.651	-17.904	1.00	145.06
	7348	CB ·	THR E		-21.783 -23.138	65.851 65.100	-19.186	1.00	145.06
5	7349	OG1	THR E		-24.059	65.683	-19.247 -18.316	1.00	246.19
_	7350	CG2	THR E		-22.944	63.634	-18.897	1.00	246.19
	7351	C	THR E		-22.032	67.345	-19.332	1.00 1.00	246.19
	7352	0	THR E		-22.255	68.039	-18.337	1.00	145.06 145.06
10	7353	N	GLY E	153	-21.984	67.845	-20.562	1.00	193.40
10	7354	CA	GLY E	153	-22.209	69.263	-20.777	1.00	193.40
	7355	C	GLY E	153	-22.478	69.578	-22.227	1.00	193.40
	7356 7357	0	GLY E	153	-22.181	68.768	-23.105	1.00	193.40
	7358	N CA	LYS E	154	-23.044	70.751	-22.486	1.00	120.13
15	7359	CB	LYS E	154 154	-23.331 -24.722	71.135	-23.857	1.00	120.13
	7360	CG	LYS E	154	-25.193	71.763 72.073	-23.950 -25.366	1.00	168.61
	7361	CD	LYS E	154	-26.607	72.634	-25.316	1.00 1.00	168.61
	7362	CE	LYS E	154	-27.120	73.053	-26.682	1.00	168.61 168.61
20	7363	NZ	LYS E	154	-28.455	73.682	-26.542	1.00	168.61
20	7364	Ç	LYS E	154	-22.271	72.122	-24.309	1.00	120.13
	7365	o O	LYS E	154	-21.969	73.090	-23.596	1.00	120.13
	7366 7367	N CA	VAL E	155	-21.685	71.856	-25.475	1.00	169.05
	7368	CB	VAL E	155	-20.666	72.731	-26.041	1.00	169.05
25	7369	CG1	VAL E	155 . 155	-19.362 -18.328	71.985 72.927	-26.310	1.00	148.26
	7370	CG2	VAL E	155	-18.847	71.420	-26.910 -25.025	1.00	148.26
	7371	C	VAL E	155	-21.235	73.223	-27.351	1.00 1.00	148.26 169.05
	7372	0	VAL E	155	-21.684	72.425	-28.174	1.00	169.05
20	7373	Ņ	TRP E	156	-21.207	74.537	-27.537	1.00	249.39
30	7374	CA	TRP E	156	-21.767	75.132	-28.733	1.00	249.39
	7375 7376	CB	TRP E	156	-21.199	74.494	-29.991	1.00	249.75
	7376 7377	CG CD2	TRP E	156	-19.797	74.775	-30.144	1.00	249.75
	7378	CE2	TRP E	156 156	-19.204 -17.813	76.069 75.880	-30.193	1.00	249.75
35	7379	CE3	TRP E	156	-19.720	73.860 77.368	-30.292 -30.164	1.00 1.00	249.75
	7380	CD1	TRP E	156	-18.784	73.875	-30.220	1.00	249.75 249.75
	7381	NE1	TRP E	156	-17.583	74.533	-30.307	1.00	249.75
	7382	CZ2	TRP E	156	-16.919	76.947	-30.375	1.00	249.75
40	7383 7384	CZ3 CH2	TRP E	156	-18.838	78.426	-30.229	1.00	249.75
70	7385	Cn2 C	TRP E	156	-17.440	78.210	-30.344	1.00	249.75
	7386	ŏ	TRP E	156 156	-23.225 -24.004	74.814 75.512	-28.688	1.00	249.39
	7387	Ň	GLN E	157	-23.571	73.711	-28.053 -29.338	1.00 1.00	249.39
4-	7388	CA	GLN E	157	-24.945	73.299	-29.404	1.00	249.35 249.35
45	7389	CB	GLN E	157	-25.559	73.927	-30.645	1.00	249.42
	7390	cc	GLN E	157	-25.723	75.415	-30.458	1.00	249,42
	7391	CD	GLN E	157	-26.491	75.691	-29.186	1.00	249.42
	7392 7393	OE1 NE2	GLN E	157	-27.538	75.108	-28.977	1.00	249.42
50	7394	C	GLN E	157	-25.980 -25.152	76.575	-28.340	1.00	249.42
	7395	ŏ	GLN E	157	-26.238	71.797 71.302	-29.367 -29.670	1.00	249.35
	7396	N	LEU E	158	-24.109	71.074	-28.973	1.00 1.00	249.35 232.10
	7397	CA	LEU E	158	-24.192	69.626	-28.872	1.00	232.10
55	7398	ÇB	LEU E	158	-23.321	68.956	-29.935	1.00	212.17
55	7399	CG	LEU E	158	-23.853	68.895	-31.367	1.00	212.17
	7400 7401	CD1	LEU E	158	-23.486	67.531	-31.928	1.00	212.17
	7402	CD2 C	LEU E	158	-25.370	69.079	-31.415	1.00	212.17
	7403	ŏ	LEU E	158 158	-23.788 -23.007	69.124	-27.492	1.00	232.10
60	7404	Ň	ASP E	159	-24.333	69.767 67.969	-26.784	1.00	232.10
	7405	CA	ASP E	159	-24.058	67.353	-27.122 -25.830	1.00 1.00	245.44
	7406	CB	ASP E	159	-25.270	66.525	-25.381	1.00	245.44 211.53
	7407	CG	ASP E	159	-26.567	67.329	-25.373	1.00	211.53
65	7408	OD1	ASP E	159	-26.659	68.326	-24.626	1.00	211.53
UJ	7409	OD2	ASP E	159	-27.502	66.961	-26.118	1.00	211.53
	7410 7411	C O	ASP E	159	-22.822	66.454	-25.908	1.00	245.44
	7412	N	ASP E TYR E	159	-22.578	65.818	-26.936	1.00	245.44
	7413	CA CA	TYR E	160 160	-22.046 -20.842	66.411 65.570	-24.824 -24.750	1.00	168.54
70	7414	CB	TYR E	160	-19.592	65.579 66.368	-24.759 -25.140	1.00	168.54
						00.000	-20.140	1.00	216.78

	7415	CG	TYR E	160	-19.684	67.078	-26.461	1.00	216.78
	7416 7417	CD1 CE1	TYR E	160	-20.168	68.381	-26.533	1.00	216.78
	7417 7418	CD2	TYR E	160 160	-20.270	69.041	-27.747	1.00	216.78
5	7419	CE2	TYR E	160	-19.301 -19.401	66.446 67.0 9 7	-27.644 -28.868	1.00	216.78
_	7420	CZ	TYR E	160	-19.887	68.395	-28.909	1.00 1.30	216.78
	7421	ОН	TYR E	160	-20.003	69.045	-30.114	1.00	216.78 216.78
	7422	С	TYR E	160	-20.609	64.973	-23.383	1.00	168.54
10	7423	0	TYR E	160	-20.898	65.581	-22.351	1.00	168.54
10	7424	N	GLU E	161	-20.048	63.771	-23.399	1.00	118.65
	7425 7426	CA CB	GLU E	161	-19.738	63.004	-22.200	1.00	118.65
	7426 7427	CB CG	GLU E	161	-20.378	61.624	-22.330	1.00	174.81
	7428	CD	GLU E	161 161	-20.107 -21.068	60.665 59.496	-21.205 -21.241	1.00	174.81
15	7429	OE1	GLU E	161	-20.765	58.447	-20.632	1.00 1.00	174.81
	7430	OE2	GLU E	161	-22,138	59.638	-21.876	1.00	174.81 174.81
	7431	С	GLU E	161	-18.214	62.890	-22.087	1.00	118.65
	7432	0	GLU E	161	-17.529	62.655	-23.085	1.00	118.65
20	7433	N	SER E	162	-17.688	63.066	-20.877	1.00	111.13
20	7434	CA	SER E	162	-16.249	63.005	-20.643	1.00	111.13
	7435	CB	SER E	162	-15.864	63.955	-19.512	1.00	104.26
	7436 7437	OG C	SER E SER E	162	-16.548	63.616	-18.315	1.00	104.26
	7438	ŏ	SER E	162 162	-15.790 -16.609	61.603	-20.296	1.00	111.13
25	7439	Ň	GLU E	163	-14.478	60.725 61.391	-20.057	1.00	111.13
	7440	ĊA	GLU E	163	-13.915	60.079	-20.272 -19. 94 3	1.00 1.00	89.90
	7441	СВ	GLU E	163	-12.417	60.050	-20.253	1.00	89.90 240.41
	7442	CG	GLU E	163	-12.072	59.972	-21.731	1.00	240.41
	7443	CD	GLU E	163	-12.359	58.606	-22.321	1.00	240.41
30	7444	OE1	GLU E	163	-11.812	57.609	-21.802	1.00	240.41
	7445	OE2	GLU E	163	-13.128	58.527	-23.303	1.00	240.41
	7446 7447	C	GLU E	163	-14.131	59.856	-18.455	1.00	89.90
	7447 7448	0 N	GLU E PRO E	163 164	-14.028	60.795	-17.668	1.00	89.90
35	7449	CD	PRO E	164	-14.433 -14.576	58.609 57.360	-18.041	1.00	64.59
	7450	CA	PRO E	164	-14.639	58.395	-18.788 -16.606	1.00 1.00	100.06
	7451	CB	PRO E	164	-15.248	57.008	-16.568	1.00	64.59 100.06
	7452	CG	PRO E	164	-14.564	56.333	-17.682	1.00	100.06
40	7453	С	PRO E	164	-13.327	58.488	-15.846	1.00	64.59
40	7454	0	PRO E	164	-12.243	58.317	-16.415	1.00	64.59
	7455	N	LEU E	165	-13.405	58.777	-14.554	1.00	77.47
	7456 7457	CA CB	LEU E	165	-12.197	58.901	-13.758	1.00	77.47
	7457 7458	CG	LEU E	165	-11.771	60.364	-13.685	1.00	63.52
45	7459	CD1	LEU E	165 165	-10.647 -9.568	60.607 59.589	-12.688 -12.978	1.00	63.52
	7460	CD2	LEU E	165	-10.088	61.981	-12.800	1.00 1.00	63.52
	7461	C	LEU E	165	-12.415	58.362	-12.360	1.00	63.52 77.47
	7462	0	LEU E	165	-13.328	58.803	-11.665	1.00	77.47
50	7463	N	ASN E	166	-11.580	57.407	-11.959	1.00	93.16
50	7464	CA	ASN E	166	-11.684	56.801	-10.635	1.00	93.16
	7465	CB	ASN E	166	-11.050	55.421	-10.614	1.00	96.38
	7466 7467	CG OD1	ASN E	166	-12.037	54.314	-10.900	1.00	96.38
	7468	ND2	ASN E ASN E	166	-13.220	54.408	-10.581	1.00	96.38
55	7469	C	ASN E	166 166	-11.534 -10.999	53.242 57.532	-11.486	1.00	96.38
	7470	ŏ	ASN E	166	-9.975	57.633 58.232	-9.582 -9.837	1.00	93.16
	7471	Ñ	ILE E	167	-11.544	57.639	- 9 .837 -8.380	1.00 1.00	93.16 64.50
	7472	CA	ILE E	167	-10.971	58.424	-7.303	1.00	64.50
60	7473	CB	ILE E	167	-11.751	59.709	-7.114	1.00	67.49
60	7474	CG2	ILE E	167	-11.452	60.314	-5.762	1.00	67.49
	7475	CG1	ILE E	167	-11.427	60.672	-8.243	1.00	67.49
	7476 7477	CD1	ILE E	167	-12.043	62.011	-8.046	1.00	67.49
	7477 7478	C O	ILE E	167	-11.054	57.651	-6.012	1.00	64.50
65	7479	Ň	THR E	167 168	-12.117	57.081	-5.675	1.00	64.50
	7480	CA	THR E	168	-9.963 -9.997	57.632 56.899	-5.266	1.00	85.23
	7481	CB	THR E	168	-9.077	55.692	-4.025 -4.075	1.00	85.23
	7482	OG1	THR E	168	-9.470	54.848	-5.162	1.00 1.00	118.46 118.46
70	7483	CG2	THR E	168	-9.178	54.910	-2.787	1.00	118.46
70	7484	С	THR E	168	-9.621	57.759	-2.856	1.00	85.23

	7400	_							
	7485	0	THR E	168	-8.681	58.558	-2.931	1.00	85.23
	7486	N	VAL E	169	-10.379	57.600	-1.781	1.00	
	7487	CA.	VAL E	169	-10.150	58.320	-0.544	1.00	97.28
_	7488	CB .	VAL E	169	-11.420	59.087	-0.122		97.28
5	7489	CG1	VAL E	169	-11.346	59.434		1.00	79.18
	7490	CG2	VAL E	169	-11.565	60.340	1.333	1.00	79.18
	7491	Č	VAL E	169			-0.927	1.00	79.18
	7492	ŏ			-9.809	57.241	0.489	1.00	97.28
	7493		VAL E	169	-10.681	56.475	0.905	1.00	97.28
10		N	ILE E	170	-8.538	57.156	0.876	1.00	87.96
10	7494	CA	ILE E	170	-8.113	56.159	1.856	1.00	87.96
	7495	CB	ILE E	170	-6.663	55.682	1.574	1.00	
	7496	CG2	ILE E	170	-6.530	55.259	0.124	1.00	99.84
	7497	CG1	ILE E	170	-5.666	56.808	1.822		99.84
	7498	CD1	ILE E	170	-4.217	56.427		1.00	99.84
15	7499	C	ILE E	170	-8.209		1.528	1.00	99.84
	7500	ŏ	ILE E			56.759	3.253	1.00	87. 96
	7501	Ň		170	-8.544	57.933	3.392	1.00	87.96
			LYS E	171	-7.932	55.970	4.286	1.00	171.73
	7502	CA	LYS E	171	-8.001	56.486	5.650	1.00	171.73
20	7503	CB	LYS E	171	-9.242	55.^^3	6.353	1.00	217.19
20	7504	ÇG	LYS E	171	-9.308	54.421	6.380	1.00	217.19
	7505	CD	LYS E	171	-10.739	53.932	6.537	1.00	217.19
	7506	CE	LYS E	171	-11.376	54.437	7.821	1.00	
	7507	NZ	LYS E	171	-12.786	53.971	7.947		217.19
	7508	С	LYS E	171	-6.749	50.162		1.00	217.19
25	7509	· ŏ	LYS E	171	-6.573		6.454	1.00	171.73
	7510	Č1	NAG E			56.658	7.565	1.00	171.73
	7511	C2		221	0.947	78.578	-23.161	1.00	249.29
	7512		NAG E	221	-0.412	79.265	-23.224	1.00	249.29
		N2	NAG E	221	-1.456	78.261	-23.255	1.00	249.29
30	7513	C7	NAG E	221	-2.671	78.553	-22.807	1.00	249.29
30	7514	07	NAG E	221	-2.963	79.651	-22.339	1.00	249.29
	7515	C8	NAG E	221	-3.720	77.456	-22.880	1.00	249.29
	7516	СЗ	NAG E	221	-0.518	80.128	-24.473	1.00	249.29
	7517	O3	NAG E	221	-1.714	80.890	-24.425	1.00	
	7518	C4	NAG E	221	0.670	81.073	-24.631	1.00	249.29
35	7519	O4	NAG E	221	0.579	81.653	-25.947	1.00	249.29
	7520	C5	NAG E	221	1.997	80.296	-24.470		249.29
	7521	O5	NAG E	221	1.994	79.555	-23.228	1.00	249.29
	7522	C6	NAG E	221	3.222	81.198	-24.429	1.00	249.29
	7523	06	NAG E	221	3.160	82.105		1.00	249.29
40	7524	C1	NAG E	222	1.316		-23.335	1.00	249.29
	7525	C2	NAG E	222		82.790	-26.227	1.00	249.77
	7526	N2	NAG E	222	0.449	83.797	-27.008	1.00	249.77
	7527	C7	NAG E		-0.713	84.171	-26.221	1.00	249.77
	7528	07 07		222	-0.903	85.441	-25.867	1.00	249.77
45	7529	C8	NAG E	222	-0.130	86.350	-26.178	1.00	249.77
73	7530		NAG E	222	-2.140	85.750	-25.043	1.00	249.77
		C3	NAG E	222	0.003	83.194	-28.351	1.00	249.77
	7531	O3	NAG E	222	-0.664	84.182	-29.124	1.00	249.77
	7532	C4	N/.G E	222	1.211	82.656	-29.133	1.00	249.77
50	7533	O4	NAG E	222	0.762	81.952	-30.285	1.00	249.77
50	7534	C5	NAG E	222	2.048	81.716	-28.248	1.00	249.77
	7535	O 5	NAG E	222	2.440	82.386	-27.023	1.00	
	7536	C6	NAG E	222	3.319	81.240	-28.926		249.77
	7537	O6	NAG E	222	3.494	79.843	-28.749	1.00	249.77
	7538	C1	NAG E	242	6.691	58.325		1.00	249.77
55	7539	C2	NAG E	242			-21.511	1.00	184.18
	7540	N2	ijis E	242	6.772	58.888	-22.927	1.00	184.18
	7541	C7			7.616	60.057	-22.949	1.00	184.18
	7542	07 07	NAG E	242	8.669	60.081	-23.755	1.00	184.18
	7543		NAG E	242	8.972	59.137	-24.489	1.00	184.18
60		C8	NAG E	242	9.523	61.338	-23.746	1.00	184.18
w	7544	C3	NAG E	242	5.382	59. 26 4	-23.429	1.00	184.18
	7545	03	NAG E	242	5.460	59.693	-24.778	1.00	184.18
	7546	C4	NAG E	242	4.452	58.056	-23.332	1.00	184.18
	7547	04	NAG E	242	3.102	58.481	-23.616	1.00	
	7548	CS	NAG E	242	4.513	57.446	-21.911		184.18
65	7549	O5	NAG E	242	5.874	57.166	-21.520	1.00	184.18
	7550	C6	NAG E	242	3.835	58.114		1.00	184.18
	7551	06	NAG E	242	2.768		-21.900	1.00	184.18
	7552	C1	NAG E	243	2.700	56.046 57.010	-20.979	1.00	184.18
	7553	ÇŞ	NAG E	243		57.919 57.901	-24.745	1.00	162.87
70	7554	N2	NAG E	243	0.990	57.891	-24.616	1.00	162.87
			1000 L	£+0	0.580	57.065	-23.493	1.00	162.87
						-			

	7555	C 7	NAG E	243	-0.334	57.510	-22.639	1.00	
	7556	07	NAG E	243	-0.848	58.623	-22.639 -22.738	1.00 1.00	162.87
	7557	C8	NAG E	243	-0.729	56.592	-21.497	1.00	162.87 162.87
_	7558	C3	NAG E	243	0.393	57.321	-25.904	1.00	162.87
5	7559	03	NAG E	243	-1.018	57.363	-25.842	1.00	162.87
	7560 7561	C4	NAG E	243	0.891	58.108	-27.133	1.00	162.87
	7561 7562	O4 C5	NAG E	243	0.428	57.479	-28.366	1.00	162.87
	7563	O5	NAG E NAG E	243 243	2.430 2.904	58.133	-27.118	1.00	162.87
10	7564	C6	NAG E	243	3.044	58.707 58.927	-25.885	1.00	162.87
	7565	06	NAG E	243	2.770	60.311	-28.250 -28.097	1.00 1.00	162.87
	7566	C1	MAN E	244	-0.169	58.185	-29.362	1.00	162.87
	7567	C2	MAN E	244	-1.467	58.963	-29.047	1.00	177.48 177.48
1.5	7568	O2	MAN E	244	-1.159	60.326	-28.837	1.00	177.48
15	7569	C3	MAN E	244	-2.273	58.794	-30.382	1.00	177.48
	7570	O3	MAN E	244	-3.531	59.444	-30.342	1.00	177.48
	7571 7572	C4 O4	MAN E	244	-1.469	59.230	-31.646	1.00	177.48
	7573	C5	MAN E MAN E	244 244	-2.267 -0. 22 3	59.074	-32.823	1.00	177.48
20	7574	O5	MAN E	244	0.620	58.317 58.472	-31.725	1.00	177.48
_ •	7575	C6	MAN E	244	0.611	58.487	-30.547 -33.000	1.00 1.00	177.48
	7576	O 6	MAN E	244	1.488	59.592	-32.913	1.00	177.48
	7577	C1		250	13.381	78.909	-13.725	1.00	177.48 249.71
0.5	7578	C2	NAG E	250	12.909	80.209	-13.049	1.00	249.71
25	7579	N2	NAG E	250	13.077	80.124	-11.608	1.00	249.71
	7580	C7	NAG E	250	13.987	80.876	-10.993	1.00	249.71
	7581 7582	O7	NAG E	250	14.727	81.658	-11.592	1.00	249.71
	7583	C8 C3	NAG E NAG E	250	14.097	80.733	-9.481	1.00	249.71
30	7584	03	NAG E	250 250	11.429 11.000	80.446 81.693	-13.387	1.00	249.71
	7585	C4	NAG E	250	11.216	80.427	-12.858 -14.906	1.00 1.00	249.71
	7586	04	NAG E	250	9.826	80.512	-15.194	1.00	249.71 249.71
	7587	C5	NAG E	250	11.793	79.133	-15.504	1.00	249.71
25	7588	O 5	NAG E	250	13.187	78.993	-15.143	1.00	249.71
35	7589	C6	NAG E	250	11.720	79.107	-17.018	1.00	249.71
	7590 7591	O6	NAG E	250	12.531	78.071	-17.553	1.00	249.71
	7592	C1 C2	NAG E NAG E	274 274	17.952 17.034	58.017	0.947	1.00	232.95
	7593	N2	NAG E	274	16.704	57.505 58.587	2.065 2.972	1.00	232.95
40	7594	C7	NAG E	274	15.587	58.533	2.972 3.690	1.00 1.00	232.95 232.95
	7595	07	NAG E	274	14.789	57.594	3.617	1.00	232.95
	7596	C8	NAG E	274	15.307	59.699	4.627	1.00	232.95
	7597	C3	NAG E	274	17.729	56.379	2.842	1.00	232.95
45	7598	03	NAG E	274	16.822	55.816	3.780	1.00	232.95
45	7599 7600	C4 O4	NAG E	274	18.227	55.288	1.888	1.00	232.95
	7601	C5	NAG E NAG E	274 274	18.999	54.339	2.613	1.00	232.95
	7602	O5	NAG E	274	19.081 18.329	55.909 56.933	0.772	1.00	232.95
	7603	C6	NAG E	274	19.520	54.898	0.083 -0.274	1.00 1.00	232.95
50	7604	O6	NAG E	274	20.106	55.536	-1.399	1.00	232.95 232.95
	7605	C1	NAG E	335	-12.841	75.891	-12.527	1.00	244.27
	7606	C2	NAG E	335	-11.869	76.721	-11.656	1.00	244.27
	7607	N2	NAG E	335	-12.291	76.605	-10. 27 1	1.00	244.27
55	7608 7609	C7	NAG E	335	-11.503	76.035	-9.365	1.00	244.27
55	7610	O7 C8	NAG E NAG E	225	-10.386	75.589	-9.628	1.00	244.27
	7611	C3	NAG E	335 335	-12.039 -11.803	75.956 78.214	-7.947	1.00	244.27
	7612	03	NAG E	335	-10.618	78.779	-12.025 -11.480	1.00	244.27
	7613	C4	NAG E	335	-11.806	78.418	-13.537	1.00 1.00	244.27 244.27
60	7614	O 4	NAG E	335	-11.818	79.805	-13.844	1.00	244.27
	7615	C5	NAG E	335	-13.044	77.739	-14.108	1.00	244.27
	7616 7647	O5	NAG E	335	-12.940	76.310	-13.913	1.00	244.27
	7617 7618	C6	NAG E	335	-13.184	77.982	-15.605	1.00	244.27
65	7618 7619	O6 C1	NAG E NAG E	335 340	-14.397	78.652	-15.913	1.00	244.27
-	7620	C2	NAG E	340	-14.368 -13.779	66.477 65.340	8.751	1.00	249.77
	7621	N2	NAG E	340	-13.779	65.349 64.233	9.574 8.721	1.00	249.77
	7622	C7	NAG E	340	-12.195	63.711	8.818	1.00 1.00	249.77 249.77
70	7623	07	NAG E	340	-11.344	64.132	9.612	1.00	249.77
70	7624	C8	NAG E	340	-11.863	62.550	7.900	1.00	249.77
								· -	

5	7625 7626 7627 7628 7629	C3 O3 C4 O4 C5	NAG E NAG E NAG E	340 -14.783 340 -14.195 340 -15.166 340 -16.238	64.920 63.909 66.132 65.759	10.636 11.453 11.500 12.355	1.00 1.00 1.00	249.77 249.77 249.77
10	7630 7631 7632 7633 7634 7635 7636	O5 C6 O6 C1 C2 N2	NAG E NAG E NAG E NAG E NAG E NAG E	340 -15.575 340 -14.610 340 -15.666 340 -15.300 366 -12.398 366 -11.828 366 -11.760	67,356 67,605 68,648 69,781 52,150 51,489 52,463	10.636 9.591 11.433 10.659 -11.858 -13.095	1.00 1.00 1.00 1.00 1.00 1.00	249.77 249.77 249.77 249.77 249.77 131.22 131.22
15	7637 7638 7639 7640 7641 7642	C7 O7 C8 C3 O3 C4	NAG E NAG E NAG E NAG E NAG E	366 -10.652 366 -9.658 366 -10.642 366 -12.712 366 -12.088 366 -12.958	53.170 53.028 54.189 50.337 49.646 49.373	-14.162 -14.339 -13.631 -15.474 -13.517 -14.588	1.00 1.00 1.00 1.00 1.00 1.00	131.22 131.22 131.22 131.22 131.22 131.22
20	7643 7644 7645 7646 7647	O4 C5 O5 C6 O6 C1	NAG E NAG E NAG E NAG E NAG E NAG E	366 -13.982 366 -13.414 366 -12.496 366 -13.478 366 -13.939	48.430 50.137 51.204 49.261 49.998	-12.351 -12.735 -11.096 -10.795 -9.862 -8.740	1.00 1.00 1.00 1.00 1.00	131.22 131.22 131.22 131.22 131.22
25	7648 7649 7650 7651 7652	C2 N2 C7 O7 C8	NAG E NAG E NAG E NAG E NAG E	367 -13.682 367 -14.975 367 -15.776 367 -16.904 367 -17.315 367 -17.698	47.077 46.261 46.701 47.372 47.646	-12.614 -12.520 -11.394 -11.610 -12.739	1.00 1.00 1.00 1.00 1.00	131.22 245.35 245.35 245.35 245.35
30	7653 7654 7655 7656 7657	C3 O3 C4 O4 C5	NAG E NAG E NAG E NAG E NAG E	367 -14.620 367 -15.804 367 -13.757 367 -13.340	47.808 44.778 43.995 44.354 43.005	-10.389 -12.391 -12.351 -13.584 -13.423	1.00 1.00 1.00 1.00 1.00	245.35 245.35 245.35 245.35 245.35
35	7658 7659 7660	O5 C6 O6	NAG E NAG E NAG E	367 -12.529 367 -12.935 367 -11.710 367 -11.792	45.270 46.662 44.973 46.031	-13.701 -13.772 -14.941 -15.884	1.00 1.00 1.00 1.00	245.35 245.35 245.35 245.35 245.35

Table 6. Atomic coordinates of PhFcεRIα₁₋₁₇₂, Form T2

			uman	es of	PhFceRi	α ₁₋₁₇₂ , Forn	n TO			
<u>at</u> Nu		TOM	ESIDUE							
_ 1		_			X_	- <u>Y</u>	_	Z		,
5 2	C	_	S C	4	16.063		•		<u>occ</u>	B
3	Ċ		'S C	4	17.178			50.293	1.00	
4	Ci	E LY	S C	4	18.081	44.372 43.766		49.692	1.00	240.56
5 6	N2			4 4	19.152	42.864		50.766	1.00	240.56 240.56
10 7	C	LY		4	20.054	42.261		50.151 51.173	1.00	240.56
8	0 N	LY:	s c	4	14.440 14.364	44.631		8.479	1.00	240.56
9	CA	LYS	S C	4	14.039	43.506		8.972	1.00 1.00	248.46
10	N	PRO	3 C	4	15.077	46.614 45.783	4	9.935	1.00	248.46 248.46
15 11	CD	PRO	ÖC	5 5	13.962	44.902		9.257	1.00	248.46
13	CA CB	PRO) C	5	13.761 13.338	46.229		7.256 5.635	1.00	240.49
14	CG	PRO) C	5	12.401	43.853		3.448	1.00 1.00	226.60
15	č	PRO PRO	0.0	5	13.189	44.636 45.881	45	.543	1.00	240.49
20 ¹⁶	0	PRO		5 5	14.379	43.053	45	.274	1.00	226.60 226.60
18	N	LYS	č	6	15.487	43.534			1.00	240.49
19	CA CB	LYS	С	6	14.022 14.932	41.831		000	1.00	240.49
20	CG	LYS LYS	C	6	15.670	40.986 40.017	44.	518	1.00 1.00	200.38
25 21	CD	LYS	C	6	16.701	39.153	45.	446 1	.00	200.38
23 22 23	CE	LYS	č	6 6	17.530	38.312	44.7	729 1	.00	249.33 249.33
24	NZ C	LYS	C	6	18.564 19.471	37.480	45.6 44.9	'	.00	249.33
25	ŏ	LYS	Ç	6	14.168	36.732	45.8	55 1	.00 .00	249.33
30 ²⁶	N	LYS VAL	_	6	13.352	40.207 39.327	43.4	49 1.	00	249.33
30 27 28	CA	VAL			14.451	40.538	43.7	55 1.	00	200.38 200.38
29	CB	VAL	9	_	13.799 14.155	39.902	42.1: 41.0:		00	184.84
30	CG1 CG2	VAL	7	,	13.207	40.623	39.74	14 17		184.84
35 32	C	VAL (?		14.108	40.181 42.134	38.64	15 1.0		175.84 175.04
<i>33</i> 32 33	0	VAL C	7		4.153	38.431	39.94	1.0	Ю	175.84 175.84
34	N CA	SER C		•	5.316 3.132	38.073	40.88 40.74	, ,,,		184.84
35	CB	SER C	۰	•	3.318	37.584	40.88			184.84
40 36 37	ÖĞ	SER C	_	1,	2.487	36.148 35.385	40.72	0 1 ດ	^	212.94
40 37 38	C	SER C	8 8	1	1.148	35.858	41.758	1.00)	212.94 203.15
39	0 N	SER C	8		2.886 2.169	35.755	41.801 39.307)	203.15
40	CA	LEU C	9		3.330	36.508	38.646		. '	212.94
45 42	СВ	TEN C	9		.955	34.593 34.137	38.834	1.00	•	212.94
43 42 43	ÇG	LEU C	9 9		.150	34.163	37.495	1.00	•	249.13 249.13
44	CD1	LEU C	9		.916	35.465	36.540 36.269	1.00		43.92
45	CD2 C	LEU C	9		.771 .966	35.258	35.022	1.00 1.00	1	43.92
50 46	ŏ	FEN C	9	12.	395	36.637 32.728	36.063	1.00	1	43.92
3U 47 48	N.	ASN C	9 10	12.	617	31.964	37.507	1.00	2	43.92 49.13
49	CA CB	ASN C	10	11. 11.	667 005	32.389	38.445 36.451	1.00	2	49.13
50	CG	ASN C	10			31.064	36.326	1.00 1.00	17	71.60
55 51 52	OD1	ASN C ASN C	10		100	30.927 29.487	37.201	1.00	17	71.60
55 52 53	ND2	ASN C	10 10	10.1	63	28.684	37.375	1.00	22	26.23 26.23
54	CO	ASN C	10	8.2 10.7	51	29.146	37.948 36.870	1.00	22	6.23
55	N	ASN C	10	9.8	'	30.744	34.882	1.00 1.00	22	6.23
60 56 57	CD	PRO C	11	11.4	'	31.353 29.806	34.315	1.00	17	1.60
9U 57 58	CA	PRO C	11	11.1	53	9.449	34.238	1.00		1.60 2.18
59	CB	PRO C	11 11	12.5	21 2	8.981	32.850 34.761	1.00		1.79
60	CG C	PRO C	11	13.02		8.248	33.517	1.00	202	2.18
65 61 62	ŏ	PRO C PRO C	11	13.68	-	8.086 9.788	32.742	1.00 1.00	161	
63 63	N	PRO C	11	13.75	3 3	9.788 1.010	35.394	1.00	161 202	
64	CD	PRO C	12 12	14.59	8 29	9.101	35.265 36.104	1.00	202	
65	CA CB	PRO C	12	14.56 15.72		.680	36.472	1.00	182.	.42
		PRO C	12	16.30).778 j.681	36.762	1.00 1.00	171.	
			•	-	40	.001	37.663	1.00	182. 171.	42 80
									171.	50

	136 137	CB CG	GLU C	20 ·	12.136	30.161	25.259	1.00	176.57
	138	CD	GLU C	20	12.994	29.290	24.335	1.00	176.57
	139	OE1 ·	GLU C	20 20	14.115 14.898	28.594	25.077	1.00	176.57
5	140	OE2	GLU C	20	14.217	29.282 27.356	25.777	1.00	176.57
	141	C	GLU C	20	10.297	31.833	24.959 25.582	1.00	176.57
	142	0	GLU C	20	10.532	33.032	25.419	1.00 1.00	154.05
	143	N	ASN C	21	9.550	31.365	26.587	1.00	154.05 173.20
10	144	CA	ASN C	21	8.957	32.290	27.559	1.00	173.20
10	145	CB	ASN C	21	7.446	32.074	27.682	1.00	249.69
	146 147	CG	ASN C	21	6.794	31.675	26.378	1.00	249.69
	148	OD1 ND2	ASN C ASN C	21	7.014	32.277	25.326	1.00	249.69
	149	C	ASN C	21 21	5.961 9.559	30.647 32.227	26.472	1.00	249.69
15	150	ŏ	ASN C	21	9.892	31.148	28.975	1.00	173.20
	151	Ň	VAL C	22	9.661	33.393	29.474 29.617	1.00	173.20
	152	CA	VAL C	22	10.209	33.508	30.964	1.00 1.00	186.44
	153	CB	VAL C	22	11.664	34.016	30.926	1.00	186.44 163.28
20	154	CG1	VAL C	22	11.701	35.486	30.538	1.00	163.28
20	155	CG2	VAL C	22	12.315	33.802	32.273	1.00	163.28
	156 157	C	VAL C	22	9.379	34.489	31.797	1.00	186.44
	158	N	VAL C	22 23	8.852	35.463	31.271	1.00	186.44
	159	CA	THR C	23 23	9.289 8.512	34.241	33.102	1.00	165.76
25	160	CB	THR C	23	7.425	35.092 34.263	34.014	1.00	165.76
	161	OG1	THR C	23	6.671	33.521	34.728 33.760	1.00	249.09
	162	CG2	THR C	23	6.492	35.177	35.511	1.00 1.00	249.09
	163	С	THR C	23	9.348	35.780	35.098	1.00	249.09 165.76
20	164	0	THR C	23	10.061	35.119	35.850	1.00	165.76
30	165	N	LEU C	24	9.239	37.099	35.195	1.00	173.95
	166 167	CA	LEU C	24	9.990	37.842	36.206	1.00	173.95
	168	CB CG	LEU C	24	10.661	39.079	35.589	1.00	128.36
	169	CD1	LEU C	24 24	11.163 12.080	39.097	34.140	1.00	128.36
35	170	CD2	LEU C	24	11.903	40.307 37.824	33.939	1.00	128.36
	171	C	LEU C	24	9.089	38.297	33.821 37.365	1.00 1.00	128.36
	172	0	LEU C	24	8.276	39.207	37.208	1.00	173.95 173.95
	173	N	THR C	25	9.249	37.669	38.526	1.00	172.54
40	174	CA	THR C	25	8.463	37.995	39.717	1.00	172.54
40	175	CB	THR C	25	8.096	36.712	40.504	1.00	195.25
	176 177	OG1 CG2	THR C	25	7.369	35.824	39.645	1.00	195.25
	178	C	THR C	25 25	7.244	37.045	41.724	1.00	195.25
	179	ŏ	THR C	25 25	9.253 10.427	38.923 38.681	40.636	1.00	172.54
45	180	Ň	CYS C	26	8.610	39.978	40.895 41.130	1.00	172.54
	181	CA	CYS C	26	9.269	40.937	42.025	1.00 1.00	199.84
	182	С	CYS C	26	9.272	40.407	43.458	1.00	199.84 199.84
	183	0	CYS C	26	8.303	39.775	43.889	1.00	199.84
50	184	CB	CYS C	26	8.556	42.292	41.955	1.00	211.93
J U	185 186	SG N	CYS C	26	9.426	43.668	42.769	1.00	211.93
	187	CA CA	ASN C ASN C	27	10.358	40.673	44.186	1.00	249.36
	188	CB	ASN C	27 27	10.531 11.176	40.203	45.564	1.00	249.36
	189	čĠ	ASN C	27	11.614	41.291 40.764	46.437	1.00	249.69
55	190	OD1	ASN C	27	12.279	39.728	47.804 47.907	1.00 1.00	249.69
	191	ND2	ASN C	27	11.246	41.481	48.858	1.00	249.69 249.69
	192	Ç	ASN C	27	9.245	39.705	46.225	1.00	249.36
	193	0	ASN C	27	8.484	40.481	46.815	1.00	249.36
60	194 195	N	GLY C	28	9.029	38.395	46.116	1.00	249.69
00	196	CA C	GLY C	28	7.858	37.746	46.685	1.00	249.69
	197	ŏ	GLY C GLY C	28 28	7.872	36.313	46.199	1.00	249.69
	198	Ň	ASN C	29	7.839 7.927	36.074 35.361	44.991	1.00	249.69
	199	CA	ASN C	29	7.980	33.942	47.129 46.771	1.00	249.69
65	200	СВ	ASN C	29	8.454	33.111	46.771	1.00 1.00	249.69 249.69
	201	CG	ASN C	29	8.804	31.655	47.627	1.00	249.69 249.69
	202	OD1	ASN C	29	8.854	31.278	46.450	1.00	249.69
	203	ND2	ASN C	29	9.055	30.840	48.650	1.00	249.69
70	204 205	C	ASN C	29	6.655	33.386	46.224	1.00	249.69
, ,	200	0	ASN C	29	6.633	32.784	45.140	1.00	249.69

							10.010	1.00	240 60
	000	N	ASN C	30°	5.554	33.594	46.946	1.00 1.00	249.69 249.69
	206 207	CA	ASN C	30	4.270	33.055	46.497 47.424	1.00	249.69
	208	CB	ASN C	30	3.852	31.902	47.372	1.00	249.69
	209	ČĞ	ASN C	30	4.822	30.717 30.182	48.410	1.00	249.69
	210	OD1	ASN C	30	5.230	30.299	46.163	1.00	249.69
	211	ND2	ASN C	30	5.186	34.055	46.361	1.00	249.69
	212	C	ASN C	30	3.119 2.662	34.325	45.248	1.00	249.69
	213	0	ASN C PHE C	30 31	2.650	34.602	47.482	1.00	249.69
	214	N	PHE C PHE C	31	1.531	35.546	47.446	1.00	249.69
10	215	CA CB	PHE C	31	0.361	35.003	48.290	1.00	249.52 249.52
	216	CG	PHE C	31	-0.075	33.609	47.903	1.00 1.00	249.52 249.52
	217 218	CD1	PHE C	31	0.636	32.498	48.348 47.071	1.00	249.52
	219	CD2	PHE C	31	-1.176	33.411	47.966	1.00	249.52
15	220	CE1	PHE C	31	0.261	31.211 32.128	46.684	1.00	249.52
••	221	CE2	PHE C	31	-1.557 -0.838	31.026	47.132	1.00	249.52
	222	CZ	PHE C	31 31	1.872	36.984	47.884	1.00	249.69
	223	C	PHE C PHE C	31	2.350	37.221	49.003	1.00	249.69
00	224	0 N	PHE C	32	1.605	37.936	46.986	1.00	249.62 249.62
20	225	CA	PHE C	32	1,872	39.354	47.227	1.00 1.00	249.69
	226 227	CB	PHE C	32	2.862	39.873	46.176 46.520	1.00	249.69
	228	CG.	PHE C	32	3.487	41.203 41.325	47.611	1.00	249.69
	229	CD1	PHE C	32	4.351	42.334	45.741	1.00	249.69
25	230	CD2	PHE C	32	3.224	42.554 42.554	47.918	1.00	249.69
	231	CE1	PHE C	32	4.948 3.814	43.566	46.039	1.00	249.69
	232	CE2	PHE C PHE C	32 32	4.678	43.673	47.130	1.00	249.69
	233	cz	PHE C PHE C	32	0.569	40.161	47.176	1.00	249.62
20	234	C O	PHE C	32	-0.470	39.650	46.738	1.00	249.62 238.93
30	235	N	GLU C	33	0.636	41.424	47.595 47.631	1.00 1.00	238.93
	236 237	CA	GLU C	33	-0.554	42.273	49.079	1.00	249.69
	238	СВ	GLU C	33	-0.811	42.705 43.193	49.339	1.00	249.69
	239	CG	GLU C	33	-2.234 -3.285	42.246	48.762	1.00	249.69
35	240	CD	GLU C	33 33	-3.265 -3.144	41.010	48.947	1.00	249.69
	241	OE1	GLU C	33	-4.250	42.733	48.124	1.00	249.69
	242	OE2	GLU C	33	-0.613	43.512	46.721	1.00	238.93 238.93
	243	C	GLU C	33	-1.589	43.716	45.998	1.00 1.00	237.42
40	244 245	Ň	VAL C	34	0.420	44.344	46.762 45.959	1.00	237.42
40	246	ĊA	VAL C	34	0.452	45.563 46.350	46.235	1.00	249.69
	247	CB	VAL C	34	1.760	47.64 4	45.447	1.00	249.69
	248	CG1	VAL C	34	1.775 1.875	46.644	47.726	1.00	249.69
	249	CG2	VAL C VAL C	34 34	0.284	45.376	44.447	1.00	237.42
45	250	CO	VAL C	34	0.665	44.351	43.880	1.00	237.42 249.64
	251	N	SER C	35	-0.305	46.386	43.812	1.00 1.00	249.64
	252 253	CA	SER C	35	-0.535	46.390	42.370 42.058	1.00	249.69
	254	СВ	SER C	35	-1.976	46.787	42.327	1.00	249.69
50		OG	SER C	35	-2.186	48.165 47.409	41.729	1.00	249.64
	256	С	SER C	35 35	0.403 0.418	47.573	40.504	1.00	249.64
	257	0	SER C	36	1.171	48.101	42,573	1.00	249.69
	258	N	SER C SER C	36	2.129	49.109	42.112	1.00	249.69 249.69
E 5	259	CA CB	SER C	36	2.054	50.374	42.987	1.00 1.00	249.69
55	5 260 261	õĞ	SER C	36	2.599	50.160	44.280 42.130	1.00	249.69
	262	Č	SER C	36	3.555	48,551	43.142		249.69
	263	Ō	SER C	36	4.261	48.626 47.977	40.999		198.99
	264	N	THR C		3.961 5.286	47.408	40.863		198.99
6	0 265	CA	THR C		5.205	45.867	40.697	1.00	176.65
	266	CB	THR C			45.280	41.840		176.65
	267	OG1	THR C			45. 27 5	40.573		176.65
	268	CG2	THR C			48.053	39.632		198.99 198.99
-	269	CO	THR C		5.232	48.246	38.619		249.69
О	5 270 271	Ñ	LYS		7.182	48.400	39.723 38.606	- <u>-</u>	249.69
	271	ČA	LYS C	38		49.041 50.287	39,109		249.38
	273	СВ	LYS C				39.79		249.38
	274	CG	LYS				40.30		249.38
7	70 275	CD	LYS (<i>,</i> 30	, (1.40 1	 3:			

	276	CE	LYS C	38	7.527	53.572	40.930	1.00	249.38
	277	NZ.	LYS C	38	8.240	54.792	41.414	1.00	249.38
	278 279	C	LYS C LYS C	38	8.837	48.092	37.894	1.00	249.69
5	280	Ň	TRP C	38 39	9. 47 3 8.933	47.247 48.221	38.519	1.00	249.69
_	281	CA	TRP C	39	9.837	47,391	36.576 35.790	1.00 1.00	205.23
	282	CB	TRP C	39	9.052	46.417	34.916	1.00	205.23 163.48
	283	CG	TRP C	39	8.273	45.376	35.653	1.00	163.48
10	284	CD2	TRP C	39	8.795	44.365	36.525	1.00	163.48
10	285 286	CE2 CE3	TRP C	39	7.715	43.525	36.893	1.00	163.48
	287	CD1	TRP C	39 39	10.069 6.939	44.083 45.125	37.032 35.540	1.00	163.48
	288	NE1	TRP C	39	6.591	44.013	35.542 36.278	1.00 1.00	163.48 163.48
	289	CZ2	TRP C	39	7.866	42.419	37.737	1.00	163.48
15	290	CZ3	TRP C	39	10.225	42.976	37.881	1.00	163.48
	291 292	CH2 C	TRP C	39	9.125	42.162	38.220	1.00	163.48
	293	ŏ	TRP C	39 39	10.637 10.076	48.332 49.233	34.908	1.00	205.23
	294	ũ	PHE C	40	11.947	48.138	34.280 34.857	1.00 1.00	205.23
20	295	CA	PHE C	40	12.800	49.016	34.034	1.00	127.08 127.08
	296	CB	PHE C	40	13.686	49.895	34.930	1.00	249.69
•	297 298	CG	PHE C	40	12.922	50.766	35.900	1.00	249.69
	299	CD1 CD2	PHE C PHE C	40 40	12.431	50.242	37.097	1.00	249.69
25	300	CE1	PHE C	40	12.724 11.762	52.121 51.055	35.630	1.00	249.69
	301	CE2	PHE C	40	12.054	52.941	38.010 36.539	1.00 1.00	249.69
	302	CZ	PHE C	40	11.574	52.408	37.731	1.00	249.69 249.69
	303	C	PHE C	40	13.714	48.294	33.012	1.00	127.08
30	304 305	O N	PHE C HIS C	40	14.938	48.204	33.191	1.00	127.08
20	306	CA CA	HIS C	41 41	13.118 13.846	47.801 47.101	31.936	1.00	117.94
	307	СВ	HIS C	41	12.846	46.566	30.884 29.848	1.00 1.00	117.94 198.34
	308	CG	HIS C	41	13.482	45.817	28.723	1.00	198.34
35	30 9 310	CD2	HIS C	41	13.214	45.791	27.395	1.00	198.34
25	311	ND1 CE1	HIS C HIS C	41 41	14.515 14.856	44.930	28.924	1.00	198.34
	312	NE2	HIS C	41	14.082	44.390 44.895	27.769 26.826	1.00	198.34
	313	C	HIS C	41	14.863	48.015	30.192	1.00 1.00	198.34 117.94
40	314	0	HIS C	41	14.509	48.859	29.389	1.00	117.94
40	315 316	N CA	ASN C ASN C	42	16.135	47.813	30.481	1.00	147.15
	317	CB	ASN C	42 42	17.216 17.135	48.618 48.679	29.912	1.00	147.15
	318	CG	ASN C	42	17.652	47.411	28.370 27.699	1.00 1.00	208.25 208.25
45	319	OD1	ASN C	42	17.253	46.309	28.074	1.00	208.25
45	320 321	ND2	ASN C	42	18.527	47.562	26.702	1.00	208.25
	322	C O	ASN C ASN C	42 42	17.140	50.019	30.506	1.00	147.15
	323	Ň	GLY C	43	17.627 16.527	50.986 50.115	29.917 31.683	1.00	147.15
	324	CA	GLY C	43	16.372	51.400	32.344	1.00 1.00	230.72 230.72
50	325	Ç	GLY C	43	15.019	52.031	32.048	1.00	230.72
	326 327	0 N	GLY C	43	14.369	52.590	32.933	1.00	230.72
	328	CA	SER C SER C	44 44	14.596 13.320	51.937	30.790	1.00	208.53
	329	CB	SER C	44	13.133	52.490 52.231	30.334 28.83	1.00	208.53
55	330	OG	SER C	44	14.168	52.830	28.070	1.00 1.00	178.10 178.10
	331	C	SER C	44	12.146	51.881	31.079	1.00	208.53
	332 333	0 N	SER C	44	11.961	50.670	31.066	1.00	208.53
	334	CA	LEU C	45 45	11.338 10.186	52.719 52.014	31.713	1.00	211.15
60	335	СВ	LEU C	45	9.346	52.214 53.372	32,442 32,985	1.00 1.00	211.15
	336	CG	LEU C	45	8.132	52.948	33.821	1.00	239.89 239.89
	337	CD1	LEU C	45	8.571	52.034	34.952	1.00	239.89
	338 339	CD2	LEU C	45 45	7.433	54.178	34.368	1.00	239.89
65	340	ŏ	LEU C	45 45	9.330 9.278	51.325 51.528	31.540	1.00	211.15
	341	N	SER C	46	8.669	50.339	30.323 32.143	1.00 1.00	211.15 166.46
	342	CA	SER C	46	7.826	49.404	31.400	1.00	166.46 166.46
	343 344	CB CC	SER C	46	8.138	47.964	31.815	1.00	249.69
70	345	og C	SER C SER C	46 46	7.394 8.345	47.032	31.043	1.00	249.69
		-		₩.	6.345	49.671	31.608	1.00	166.46

34 34	7	O N CA	SER C GLU C GLU C	46 - 47 47	5.973 5.512 4.064	50.451 48.996 49.168	32.488 30.813 30.864 29.458	1.00 1.00 1.00 1.00	166.46 202.45 202.45 249.69
34 34		CB .	GLU C	47	3.485 4.000	49.010 50.047	28.469	1.00	249.69
5 35		CG	GLU C	47 47	3.429	49.860	27.078	1.00	249.69 249.69
35	51	CD	GLU C	47	3.693	48.805	26.462 26.600	1.00 1.00	249.69
35		OE1 OE2	GLU C	47	2.715	50.769	31.832	1.00	202.45
35	53 54	C	GLU C	47	3.296	48.271 48.506	32.090	1.00	202.45
	5 5	Ö	GLU C	47	2.108 3.948	47.243	32.361	1.00	214.28
	56	N	GLU C	48 48	3.264	46.372	33.301	1.00 1.00	214.28 197.36
	57	CA CB	GLU C	48	3.882	44.973	33.294 34.340	1.00	197.36
	58	CG	GLU C	48	3.286	44.027 43.715	34.097	1.00	197.36
	159 160	CD	GLU C	48	1.825 1.535	43.713 42.984	33.130	1.00	197.36
	361	OE1	GLU C	48 48	0.964	44.203	34.866	1.00	197.36 214.28
3	362	OE2	GLU C	48	3.343	46.977	34.702	1.00 1.00	214.28
	363	C O	GLU C	48	4.236	47.788	34.995 35.557	1.00	211.95
	364 365	N	THR C	49	2.398	46.584 47.069	36.932	1.00	211.95
	366	CA	THR C	49	2.335 1.126	48.003	37.123	1.00	249.69
	367	CB	THR C THR C	49 49	-0.069	47.327	36.706	1.00 1.00	249.69 249.69
	368	OG1 CG2	THR C	49	1.305	49.278	36.301 37.901	1.00	211.95
25	369	C	THR C	49	2.220	45.895 45.988	39.055	1.00	211.95
	370 371	ŏ	THR C	49	2.631 1.650	44.797	37.421	1.00	207.90
	372	N	ASN C	50 50	1.502	43.601	38.234	1.00	207.90 210.82
	373	CA	ASN C	50 50	0.856	42.486	37.403 38.245	1.00 1.00	210.82
20	374	CB CG	ASN C	50	0.443	41.295	39.365	1.00	210.82
30	375 376	OD1	ASN C	50	0.925	41.126 40.456	37.705	1.00	210.82
	377	ND2	ASN C	50 50	-0.437 2.914	43.187	38.670	1.00	207.90 207.90
	378	Ç	ASN C ASN C	50 50	3.888	43.479	37.978	1.00 1.00	249.50
~~	379	N N	SER C	51	3.036	42.509	39.808 40.286	1.00	249.50
35	380 381	CA	SER C	51	4.352	42.086 41.569	41.728	1.00	249.69
	382	CB	SER C	51	4.260 3.632	40.295	41.780	1.00	249.69
	383	ОG	SER C	51 51	4.994	41.012	39.395	1.00 1.00	249.50 249.50
	384	C	SER C	51	6.196	40.775	39.483 38.544	1.00	228.11
40	385	O N	SER C	52	4,195	40.367 39.328	37.645	1.00	228.11
	386 387	ČA	SER C	52	4.705 3.867	38.049	37.741	1.00	168.18
	388	CB	SER C	52 52		37.491	39.042		168.18 228.11
	389	OG	SER C SER C	52 52		39.783	36.194 35.528		228.11
45	390	C O	SER C	52	3.692	39.843 40.096	35,708		153.71
	391 392	Ň	LEU C			40.542	34.332	1.00	153.71
	393	CA	LEU C			41.594	34.278		123.91 123.91
	394	CB	LEU C			41.882	32.939		123.91
50	395	CG CD1	LEU		3 6.841	42.018	31.823 33.084		123.91
	396 397	CD2	LEU C		A 43A	43.157 39.373	33.43	9 1.00	153.71
	398	С	LEU () 50) 50		38.887	33.46		153.71 221.05
	399	0	LEU (38.918	32.65		221.05
55	400	N CA	ASN	C 5	4 5.772	37.804	31.77 31.43		192.59
	401 402	CB	ASN	C 5	4.474	37.081 36.312	32.60		192.59
	403	CG	ASN	C 5	3.924 4 4.626	35,511	33.21	1.00	192.59
	404	OD1	ASN	-	54 4.626 54 2.661	36.548	32.92		192.59 221.05
60	405	ND2	ASN ASN	_	6.477	38.221	30.49 30.09		221.05
	406	CO		_	54 6.451		29.8		249.69
	407 408	N	ILE	C	55 7.116		28.6	24 1.00	249.69
	409	CA	ILE	~	55 7.850 55 9.374		28.8	69 1.00	131.97 131.97
65	5 410	CB	ILE 2 ILE		55 9.374 55 10.103	36.988	27.5		404 07
	411	CG.		_	55 9.822	2 38.756	29.3 29.6		131.97
	412 413	CD.	·	C	55 11.30		27.7		249.69
	414	С	ILE	_	55 7.46 55 7.74		28.0		249.68
7	0 415	0	ILE	С	55 7.74				

					0.000	36.531	26.595	1.00	201.86
41	16	N	VAL C	58	6.829 6.422	35.474	25.687	1.00	201.86
41		CA	VAL C	56	5.043	35.759	25.089	1.00	231.54
	18	СВ	VAL C	56	4.431	34.468	24.565	1.00	231.54
	19	CG1	VAL C	56	4.144	36.385	26.138	1.00	231.54
	20	CG2	VAL C	56 56	7.454	35.345	24.578	1.00	201.86 201.86
	21	Ç	VAL C VAL C	56	8.595	35.775	24.747	1.00	157.94
4	22	0	ASN C	57	7.056	34.758	23.451	1.00 1.00	157.94
4	23	N	ASN C	57	7.953	34.542	22.310	1.00	249.57
	24	CA	ASN C	57	7.179	34.657	20.9 94 20. 793	1.00	249.57
	125	CB	ASN C	57	6.212	33.499	20.793	1.00	249.57
	126	CG OD1	ASN C	57	6.593	32.333	20.488	1.00	249.57
	127	ND2	ASN C	57	4.958	33.812	22.324	1.00	157.94
	428 428	C	ASN C	57	9.147	35.472 36.592	21.825	1.00	157.94
	429 420	ŏ	ASN C	57	9.103	34.960	22.924	1.00	146.95
	430 431	Ň	ALA C	58	10.213	35.658	23.112	1.00	146.95
	431 432	CA	ALA C	58	11.477	34.717	23.796	1.00	132.39
	433	СВ	ALA C	58	12.467	36.270	21.878	1.00	146.95
	434	С	ALA C	58	12.122 12.657	35.566	21.014	1.00	146.95
	435	0	ALA C	58	12.037	37.596	21.816	1.00	135.91
20	436	N	LYS C	59 50	12.680	38.350	20.710	1.00	135.91
	437	CA	LYS C	59 59	11.742	39.483	20.270	1.00	248.43 248.43
	438	CB	LYS C	59 59	10.375	39.002	19.795	1.00	248.43
	439	CG	LYS C	59	5.126	40.157	19.482	1.00	248.43
25	440	CD	LYS C	59	8.053	39.641	19.094	1.00	248.43
	441	CE	LYS C	59	7.100	40.738	18.771	1.00	135.91
	442	NZ	LYS C	59	13.986	38.928	21.228	1.00	135.91
	443	С	LYS C LYS C	59	14.052	39.415	22.354	1.00	130.99
	444	0	LYS C PHE C	60	15.020	38.866	20.406	1.00	130.99
30	445	N	PHE C	60	16.330	39.375	20.784	1.00 1.00	226.68
	446	CA	PHE C	60	17.171	39.581	19.523	1.00	226.68
	447	CB	PHE C	60	17.469	38.309	18.781	1.00	226.68
	448	CG	PHE C	60	17.704	38.327	17.410 19.458	1.00	226.68
	449	CD1	PHE C	60	17.535	37.093	16.724	1.00	226.68
35	450	CD2	PHE C	60	17.998	37.156	18.782	1.00	226.68
	451	CE1 CE2	PHE C	60	17.829	35.919	17.411	1.00	226.68
	452	CZ	PHE C	60	18.061	35.951	21.597	1.00	130.99
	453	C	PHE C	60	16.296	40.672	22.439	1.00	130.99
40	454	ŏ	PHE C	60	17.171	40.914	21.338	1.00	229.15
40	455	N	GLU C	61	15.289	41.507	22.028	1.00	229.15
	456	ČA	GLU C	61	15.136	42.789 43.603	21.363	1.00	236.43
	457 458	CB	GLU C	61	14.021	43.926	19.878	1.00	236.43
	450 459	CG	GLU C	61,	14.258	42.686	19.003	1.00	236.43
45	460	CD	GLU C	61	14.424 13.554	41.786	19.062	1.00	236.43
40	461	OE1	GLU C	61		42.616	18.250	1.00	236.43
	462	OE2	GLU C	61		42.608	23.508		229.15
	463	С	GLU C			43.491	24.316		229.15 169.19
	464	0	GLU C			41.456	23.849		169.19
50	465	N	ASP C			41.142	25.23		219.70
-	466	CA	ASP C			39.884	25.31		219.70
	467	CB	ASP C	62	44.057	39.951	24.41		219.70
	468	CG	ASP (6		41.064	24.22		219.70
	469	OD1	ASP (5 6	- ::	38.891	23.91		169.19
55	470	OD2	ASP (-		40.932	26.06		169.19
	471	Č	ASP (2 15.152	41.049	27.28		159.66
	472	0	SER	, e	3 16.289	40.608	25.40		159.66
	473	N	SER	C 6	3 17.564	40.400	26.08		141.40
	474	CA	SER		3 18.659	39.965	25.08		141.40
60		CB	SER		33 18.325		24.39		159.66
	476	og	SER	-	17.962	41.730	26.7		159.66
	477	C	SER		63 18.006	42.746	26.0		163.83
	478	0	GLY		64 18.242	41.730	28.0		163.83
_	_ 479	N OA	GLY	č	64 18.620	42.974	28.6		400.02
6		CA	GLY	_	64 18.666	3 42.973	30.1	·	
	481	C	GLY		64 18.65	2 41.917	30.7 30.7		4
	482	0	GLU	č	65 18.71	9 44.181	30.7 32.1		
	483	N CA	GLU	č	65 18.79	2 44.422	32.1		
_	484	CB	GLU		65 19.85	9 45.482	32.4		
1	70 485	55							

	486	CG	GLU C	65 ·	19.972	45.990	. 33.800	1.00	040.00
	487	CD	GLU C	65	20.739	47.294	33.859	1.00	246.28 246.28
	488	OE1	GLU C	65	20.270	48.276	33.250	1.00	246.28
5	489	OE2 ·	GLU C	65	21.806	47.341	34.506	1.00	246.28
J	490 491	C	GLU C	65	17.444	44.883	32.727	1.00	155.20
	492	N	GLU C TYR C	65 66	16.907	45.897	32.306	1.00	155.20
	493	CA	TYR C	66	16.899 15.614	44.149 44.507	33.692 34.299	1.00	218.21
	494	СВ	TYR C	66	14.600	43.380	34.131	1.00 1.00	218.21
10	495	CG	TYR C	66	14.195	43.050	32.722	1.00	195.34
	496	CD1	TYR C	66	15.027	42.319	31.889	1.00	195.34 195.34
	497	CE1	TYR C	66	14.607	41.929	30.619	1.00	195.34
	498 499	CD2	TYR C	66	12.934	43.398	32.250	1.00	195.34
15	500	CE2 CZ	TYR C TYR C	66	12.505	43.016	30.985	1.00	195.34
15	501	OH	TYR C	66 66	13.342 12.896	42.277	30.175	1.00	195.34
	502	Č.	TYR C	66	15.691	41.868 44.815	28.938 35.795	1.00	195.34
	503	0	TYR C	66	16.721	44.584	36.431	1.00 1.00	218.21
20	504	N	LYS C	67	14.577	45.311	36.350	1.00	218.21 178.65
20	505	CA	LYS C	67	14.467	45.652	37.782	1.00	178.65
	506	CB	LYS C	67	15.471	46.748	38.152	1.00	172.69
	507 508	CG	LYS C	67	15.399	47.981	37.275	1.00	172.69
	509	CD CE	LYS C LYS C	67 67	16.474	48.976	37.663	1.00	172.69
25	510	NZ	LYS C	67 67	16.722 17.749	50.003 51.022	36.565	1.00	172.69
	511	c	LYS C	67	13.078	46.103	36.952 38.229	1.00	172.69
	512	0	LYS C	67	12.289	46.623	37.437	1.00 1.00	178.65
	513	N	CYS C	68	12.794	45.898	39.512	1.00	178.65 193.02
20	514	CA	CYS C	68	11.523	46.307	40.083	1.00	193.02
30	515	C	CYS C	68	11.724	47.110	41.369	1.00	193.02
	516 517	O CB	CYS C	68	12.709	46.929	42.091	1.00	193.02
	518	SG	CYS C CYS C	68 68	10.604	45.104	40.336	1.00	142.23
	519	N	GLN C	69	11.079 10.780	43.935 48.008	41.620	1.00	142.23
35	520	CA	GLN C	69	10.806	48.882	41.636 42.802	1.00 1.00	226.79
	521	CB	GLN C	69	11.511	50.191	42.437	1.00	226.79 248.82
	522	CG	GLN C	69	11.193	51.363	43.344	1.00	248.82
	523	CD	GLN C	69	11.804	52.664	42.851	1.00	248.82
40	524 525	OE1 NE2	GLN C	69	11.623	53.050	41.694	1.00	248.82
40	526	C	GLN C GLN C	69 69	12.526	53.352	43.730	1.00	248.82
	527	ŏ	GLN C	69	9.370 8.470	49.163 49.208	43.221 42.382	1.00	226.79
	528	Ň	HIS C	70	9.149	49.349	44.515	1.00 1.00	226.79 241.71
4.50	529	CA	HIS C	70	7.806	49.635	45.003	1.00	241.71
45	530	CB	HIS C	70	7.524	48.852	46.292	1.00	246.85
	531	CG	HIS C	70	7.366	47.378	46.075	1.00	246.85
	532 533	CD2 ND1	HIS C	70	7.971	46.319	46.666	1.00	246.85
	534	CE1	HIS C HIS C	70 70	6.487	46.852	45.155	1.00	246.85
50	535	NE2	HIS C	70 70	u 56 7.448	45.530 45.184	45.184	1.00	246.85
	536	C	HIS C	70	7.601	51.127	46.094 45.236	1.00 1.00	246.85
	537	0	HIS C	70	8.435	51.946	44.851	1.00	241.71 241.71
	538	Ņ	GLN C	71	6.485	51.470	45.872	1.00	248.91
55	539	CA	GLN C	71	6.139	52.861	46.161	1.00	248.91
33	540 541	CB	GLN C	71	4.804	52.897	46.935	1.00	249.69
	541 542	CG	GLN C	71	4.049	54.235	46.919	1.00	249.69
	543	OE1	GLN C	71 71	3.630 3.071	54.682	45.519	1.00	249.69
	544	NE2	GLN C	71	3.889	53.904 55.949	44.741 45.201	1.00	249.69
60	545	C	GLN C	71	7.243	53.579	46.956	1.00 1.00	249.69
	546	0	GLN C	71	7.670	54.680	46.599	1.00	248.91 248.91
	547	N	GLN C	72	7.705	52.942	48.026	1.00	236.85
	548	CA	GLN C	72	8.741	53.519	48.875	1.00	236.85
65	549 550	CB	GLN C	72	8.117	53.962	50.201	1.00	249.69
UJ.	550 551	CG CD	GLN C	72 70	9.064	54.624	51.198	1.00	249.69
	552	OE1	GLN C GLN C	72 72	8.391	54.885	52.545	1.00	249.69
	553	NE2	GLN C	72 72	7.360 8.973	55.560 54.348	52.617 53.617	1.00	249.69
	554	C	GLN C	72	9.860	54.348 52.501	53.617 49.127	1.00	249.69
70	555	Ō	GLN C	72	10.188	52.301 52.188	49.127 50.274	1.00 1.00	236.85
							30.217	1.00	236.85

							40.050	1.00	249.69
			VAL C	73 ⁻	10.435	51.975	48.050	1.00	249.69
	556	N			11.519	51.001	48.163		190.27
9	557	CA	411-	73	11.016	49.546	47.988	1.00	190.27
	558	CB	**************************************	73	12.100	48.583	48.424	1.00	
	559	CG1	****	73	9.740	49.315	48.789	.1.00	190.27
	560	CG2	VAL C	73 73	12.547	51.280	47.077	1.00	249.69
•	561	С	VAL C		12.195	51.0/4	45. 96 6	1.00	249.69
	562	0	VAL C	73 74	13.819	51.080	47.397	1.00	225.53
	563	N	ASN C		14.877	51.314	46.426	1.00	225.53
	564	CA	ASN C	74 74	16.220	51.480	47.153	1.00	240.44
10	565	CB	ASN C	74 74	16.174	52.577	48.221	1.00	240.44
	566	CG	ASN C		15.597	53.643	47.999	1.00	240.44
	567	OD1	ASN C	74	16.786	52.316	49.374	1.00	240.44
	568	ND2	ASN C	74 74	14.929	50.162	45.407	1.00	225.53
	569	С	ASN C	74	14.963	48.987	45.778	1.00	225.53
15	570	0	ASN C	7 4 75	14.918	50.516	44.123	1.00	249.69
••	571	N	GLU C	75 75	14.943	49.543	43.030	1.00	249.69 249.60
	572	CA	GLU C	75 75	15.262	50.260	41.708	1.00	
	573	CB	GLU C	75 75	16.260	5134	41.834	1.00	249.60 249.60
	574	CG	GLU C	75 75	16.362	52.238	40.567	1.00	249.60
20	575	CD	GLU C	75 75	15.308	52.660	40.046	1.00	249.60
	576	OE1	GLU C	75	17.493	52.480	40.096	1.00	249.69
	577	OE2	GLU C GLU C	75	15.886	48.356	43.233	1.00	249.69
	578	Ç	GLU C	75	16.998	48.508	43.733	1.00	230.56
	579	0	SER C	76	15.421	47.175	42.830	1.00	230.56
25	580	N	SER C	76	16.178	45.932	42.968	1.00	187.63
	581	CA	SER C	76	15.307	44.734	42.596	1.00	187.63
	582	CB	SER C	76	15.123	44.661	41.190	1.00	230.56
	583	og	SER C	76	17.435	45.877	42.115	1.00	230.56
	584	Ç	SER C	76	17.565	46.600	41.124	1.00 1.00	249.20
30	585	0	GLU C	77	18.356	45.002	42.510	1.00	249.20
	586	N	GLU C	77	19.602	44.825	41.778	1.00	249.69
	587	CA	GLU C	77	20.531	43.861	42.527	1.00	249.69
	588	CB	GLU C	77	21.030	44.390	43.870	1.00	249.69
	589	CG	GLU C	77	21.895	45.639	43.734 42.611	1.00	249.69
35	590	CD OE1	GLU C	77	22.002	46.187	44.755	1.00	249.69
	591	OE2	GLU C	77	22.468	46.078	40.410	1.00	249.20
	592	_	GLU C	77	19.257	44.256	40.304	1.00	249.20
	593	C	GLU C	77	18.786	43.124	39.346	1.00	211.01
40	594	N	PRO C	78	19.492	45.042	39.342	1.00	171.69
40		CD	PRO C	78	20.275	46.292	37.977	1.00	211.01
	596	CA	PRO C	78	19.193	44.608	37.127	1.00	171.69
	597	CB	PRO C	78	20.023	45.581	37.951	1.00	171.69
	598	CG	PRO C	78	20.054	46.826	37.720	1.00	211.01
45	599	č	PRO C	78		43.155	38.420	1.00	211.01
43		ŏ	PRO C	78		42.597 42.537	36.728	1.00	200.35
	601 602	Ň	VAL C	79		42.557 41.166	36.344	1.00	200.35
	603	CA	VAL C	79		40.146	36.754	1.00	129.43
	604	CB	VAL C	79		38.805	36.090		129.43
50) 605	CG1	VAL C	79		39.966	38.259	1.00	129.43
٦,	606	CG2	VAL C	79		41.203	34.835	1.00	200.35
	607	С	VAL C			41.902	34.191		200.35
	608	Ó	VAL C	79		40.476	34.262	1.00	130.20
	609	N	TYR C		4-0	40.495	32.817	7 1.00	130.20
5	5 610	CA	TYR C	; B		40.686	32.410		206.ხა
	611	CB	TYR C	8		41.126	30.97		206.89
	612	CG	TYR C	8		42.471	30.61		206.89
	613	CD1	TYR C			42,880	29.29	0 1.00	206.89
	614	CE1	TYR	-		10.400	29.95	4 1.00	206.89
6	0 615	CD2	TYR			40.598	28.62		206.89
	616	CE2	TYR	-	·		28.29		206.89
	617	CZ	TYR				26.98	8 1.00	206.89 130.20
	618	ÓН	TYR	ָט ט ר	30 22.299 30 19.928		32.17		130.20
	619	Ç	TYR	_	BO 20.195	38.133	32.63		124.74
(65 620	0	TYR	-	81 19.172	400	31.09		124.74
•	621	N	LEU	-	81 18.624		30.39		90.50
	622	CA	LEU LEU	_	81 17.10		30.2		
	623	CB	LEU	č	81 16.47		29.4		
	624	CG			81 16.71		30.1	22 1.00	50.30
	70 625	CD1	LEU	9					

	526 527	CD2 C	LEU C	81	14.994 19.216 19.179	37.467 38.222 39.232	29.222 28.998 28.300	1.00 1.00 1.00	90.50 124.74 124.74
	828	0	LEU C	82	19.771	37.075	28.595	1.00	106.68 106.68
ا ہے	629	N ·	GLU C	82	20.322	36.967	27.253 27.305	1.00 1.00	249.60
	630 631	CB	GLU C		21.797	36.601 37.080	26.079	1.00	249.60
	632	CG	GLU C	82	22.564	36.748	26.143	1.00	249.60
	633	CD	GLU C	82 82	24.041 24.609	36.761	27.257	1.00	249.60
	634	OE1	GLU C	82	24.637	36.489	25.075	1.00	249.60 106.68
10	635	OE2 C	GLU C	82	19.546	35.917	26.454 26.994	1.00 1.00	106.68
	636 637	Ö	GLU C	82	19.224	34.834 36.244	25.186	1.00	145.59
	638	Ň	VAL C	83	19.234	35.318	24.292	1.00	145.59
	639	CA	VAL C	83	18.513 17.270	35.943	23.679	1.00	134.02
15	640	CB	VAL C VAL C	83 83	16.562	34.914	22.796	1.00	134.02 134.02
	641	CG1 CG2	VAL C	83	16.343	36.429	24.781	1.00 1.00	145.59
	642	C	VAL C	83	19.417	34.835	23.164 22.600	1.00	145.59
	643 644	ŏ	VAL C	83	20.212	35.603 33.562	22.822	1.00	150.61
20	645	N	PHE C	84	19.259	32.945	21.833	1.00	150.61
20	646	CA	PHE C	84	20.117 21.072	31.978	22.515	1.00	134.04
	647	СВ	PHE C PHE C	84 84	21.985	32.603	23.516	1.00	134.04
	648	CG	PHE C	84	21.566	32.852	24.818	1.00	134.04 134.04
0.5	649	CD1 CD2	PHE C	84	23.282	32.918	23.158	1.00 1.00	134.04
25	650 651	CE1	PHE C	84	22.433	33.403	25.743 24.078	1.00	134.04
	651 652	CE2	PHE C	84	24.151	33.468 33.712	25.370	1.00	134.04
	653	CZ	PHE C	84	23.729 19.487	32.151	20.719	1.00	150.61
	654	Ç	PHE C	84 84	18.363	31.654	20.842	1.00	150.61
30	655	0	PHE C SER C	85	20.276	31.999	19.653	1.00	176.12 176.12
	656	N CA	SER C	85	19.898	31.208	18.491	1.00 1.00	141.64
	657 658	CB	SER C	85	19.635	32.073	17.269 16.175	1.00	141.64
	659	og	SER C	85	19.275	31.250 30.334	18.214	1.00	176.12
35	660	C	SER C	85	21.092 22.171	30.838	17.876	1.00	176.12
55	661	0	SER C	85 86	20.900	29.030	18.377	1.00	126.17
	662	N	ASP C	86	21.976	28.062	18.156	1.00	126.17 148.28
	663	CA CB	ASP C	86	23.135	28.325	19.122 18.490	1.00 1.00	148.28
40	664 665	CG	ASP C	86	24.477	28.085	17.898	1.00	148.28
40	666	OD1	ASP C	86	24.674	26.995 28.999	18.587	1.00	148.28
	667	OD2	ASP C	86	25.329 21.448	26.656	18.392	1.00	126.17
	668	Ç	ASP C ASP C	86 86	20.356	26.480	18.922	1.00	126.17 154.85
	669	0 7	TRP C	87	22.220	25.650	18.003	> 1.00 1.00	154.85
45	670 671	CA	TRP C	87	21.780	24.277	18.204 17.473	1.00	249.47
	671 672	CB	TRP C	87	22.714	23.312 23.058	16.067	1.00	249.47
	673	CG	TRP C	87	22.275 22.713	23.754	14.895	1.00	249.47
	674	CD2	TRP C	87 87	22.713	23.217	13.798	1.00	249.47
50		CE2	TRP C	87	23.645	24.782	14.661	1.00	249.47 249.47
	676	CE3 CD1	TRP C	87		22.152	15.650 14.290	1.00 1.00	249.47 249.47
	677 678	NE1	TRP C	87		22.243	12.489	1.00	249.47
	679	CZ2	TRP C	87		23.670 25.232	13.361	1.00	249.47
55	680	CZ3	TRP C			24.675	12.291		249.47
	681	CH2	TRP C	87 87		23.947	19.683		154.85
	682	CO	TRP C	87		23.513	20.170		154.85 160.72
	683	Ň	LEU C		3 22.820	24.160	20.394		160.72
6	684 0 685	CA	LEU C	; 88		23.888	21.820 22.122		161.67
Ů.	686	CB	LEU C	; 81		22.726 21.360	21.543		161.67
	687	CG	LEU C			20.299	22.027	7 1.00	161.67
	688	CD1	LEU			21.001	21.96	5 1.00	161.67
_	689	CD2	LEU (_		25.124	22.62		160.72 160.72
6	5 690	CO	LEU (•	8 24.103	25.909	22.19		139.08
	691 692	N	LEU	_	9 22.613	25.306	23.78 24.65		139.08
	693	ČA	LEU (C 8	9 22.929	26.426 27.440	24.66 24.66		166.24
	694	CB	LEU		39 21.801 39 22. 04 3		25.62		166.24
7	70 695	CG	LEU	٤	39 22.043	20,000			

	696	CD1	LEU C	89	23.405	29.250	25.356	1.00	166.24
	697	CD2	LEU C	89	20.917	29.623	25.492	1.00	166.24
	698	C .	LEU C	89	23.123	25.891	26.057	1.00	139.08
5	699 700	N	LEU C	89	22.297	25.098	26.533	1.00	139.08
	701	ÇA .	LEU C	90 90	24.212 24.490	26.304 25.844	26.715	1.00	149.33
	702	CB	LEU C	90	25.993	25.806	28.077 28.323	1.00	149.33
	703	CG	LEU C	90	26.370	25.474	29.765	1.00 1.00	143.04
10	704	CD1	LEU C	90	25.808	24.104	30.144	1.00	143.04 143.04
10	705	CD2	LEU C	90	27.884	25.509	29.938	1.00	143.04
	706	C	LEU C	90	23.834	26.755	29.106	1.00	149.33
	707 708	0	LEU C	90	24.213	27.914	29.243	1.00	149.33
	708 709	N CA	GLN C GLN C	91 91	22.861	26.226	29.839	1.00	125.14
15	710	CB	GLN C	91	22.166 20.656	27.026 26.784	30.825	1.00	125.14
	711	ČĞ	GLN C	91	20.043	27.113	30.745 29.398	1.00	164.13
	712	CD	GLN C	91	18.552	26.873	29.373	1.00 1.00	164.13 164.13
	713	OE1	GLN C	91	18.078	25.769	29.661	1.00	164.13
20	714	NE2	GLN C	91	17. 79 9	27.910	29.035	1.00	164.13
20	715	C	GLN C	91	22.633	26.746	32.238	1.00	125.14
	716 717	0	GLN C	91	22.832	25.583	32.625	1.00	125.14
	718	N CA	ALA C ALA C	92	22.787	27.820	33.014	1.00	120.03
	719	CB	ALA C	92 92	23.217 24.586	27.706 28.363	34.404	1.00	120.03
25	720	č	ALA C	92	22.204	28.360	34.567 35.331	1.00	230.41
	721	ō	ALA C	92	21.618	29.392	34.993	1.00 1.00	120.03 120.03
	722	N	SER C	93	22.009	27.738	36.490	1.00	162.82
	723	CA	SER C	93	21.091	28.244	37.499	1.00	162.82
20	724	СВ	SER C	93	21.158	27.396	38.784	1.00	102.92
30	725	og	SER C	93	22.476	27.269	39.270	1.00	102.92
	726 727	C O	SER C	93	21.472	29.682	37.798	1.00	162.82
	728	N	SER C ALA C	93 94	20.699	30.618	37.567	1.00	162.82
	729	CA	ALA C	94	22.679 23.224	29.849 31.174	38.313	1.00	108.42
35	730	CB	ALA C	94	23.252	31.403	38.620 40.121	1.00 1.00	108.42
	731	C	ALA C	94	24.643	31.150	38.051	1.00	218.96 108.42
	732	0	ALA C	94	25.237	30.083	37.932	1.00	108.42
	733	N	GLU C	95	25.180	32.303	37.678	1.00	153.28
40	734	CA	GLU C	95	26.518	32.317	37.122	1.00	153.28
40	735 736	CB CB	GLU C	95	26.615	33.364	36.025	1.00	202.07
	737	CD	GLU C	95 95	25.708 25.982	33.060	34.858	1.00	202.07
	738	OE1	GLU C	95	25.862 25.257	33.949 33.821	33.677	1.00	202.07
	739	OE2	GLU C	95	26.925	34.772	32.668 33.751	1.00 1.00	202.07
45	740	C	GLU C	95	27.586	32.559	38.176	1.00	202.07 153.28
	741	0	GLU C	95	28.757	32.209	37.973	1.00	153.28
	742	N	VAL C	96	27.180	33.151	39.302	1.00	129.17
	743	CA	VAL C	96	28.105	33.428	40.407	1.00	129.17
50	744 745	CB CG1	VAL C	96	28.289	34.930	40.613	1.00	121.01
50	746	CG2	VAL C	96 96	29.526 28.379	35.175 35.630	41.441	1.00	121.01
	747	Č	VAL C	96	27.548	35.630 32.826	39.273 41.694	1.00	121.01
	748	Õ	VAL C	96	26.380	33.012	42.009	1.00 1.00	129.17
	749	N	VAL C	97	28.383	32.123	42.449	1.00	129.17 144.84
55	750	CA	VAL C	97	27.885	31.495	43.658	1.00	144.84
	751	CB	VAL C	97	27.584	30.011	43.391	1.00	123.55
	752 753	CG1 CG2	VAL C	97	26.631	29.492	44.443	1.00	123.55
	753 754	C	VAL C	97 07	27.013	29.816	42.007	1.00	123.55
60	755	ŏ	VAL C	97 97	28.756 29.987	31.574 31.649	44.921	1.00	144.84
	756	Ň	MET C	98	28.083	31.537	44.847 46.073	1.00	144.84
	757	CA	MET C	98	28.713	31.568	47.396	1.00 1.00	143.10 143.10
	758	CB	MET C	98	27.725	32.094	48.440	1.00	249.69
<i>C</i>	759	CG	MET C	98	27,288	33.530	48.256	1.00	249.69
65	760	SD	MET C	98	28.558	34.688	48.776	1.00	249.69
	761 762	CE	MET C	98	28.400	34.595	50.561	1.00	249.69
	762 763	C O	MET C	98	29.093	30.140	47.792	1.00	143.10
	764	N	MET C GLU C	98 99	28.224 30.366	29.260	47.820	1.00	143.10
70	765	CA	GLU C	99	30.817	29.905 28.560	48.115 48.495	1.00	134.64
					20.017	-	70.483	1.00	134.64

	766	СВ	GLU C	99	32,113	28.640	49.296	1.00	240.00
	767	CG	GLU C	99	32.954	27.373	49.225	1.00	249.69 249.69
	768	CD:	GLU C	99	34.077	27.361	50.242	1.00	249.69
5	769 770	OE1	GLU C	99	34.676	28.433	50.488	1.00	249.69
,	770 771	OE2 C	GLU C	99 99	34.370	26.275	50.787	1.00	249.69
	772	ŏ	GLU C	99	29.760 29.307	27.848 28.382	49.328	1.00	134.64
	773	Ň	GLY C	100	29.348	26.660	50.333 48.899	1.00	134.64
	774	CA	GLY C	100	28.349	25.925	49.654	1.00 1.00	174.64
10	775	С	GLY C	100	26.950	25.885	49.070	1.00	174.64 174.64
	776	0	GLY C	100	26.164	25.012	49.424	1.00	174.64
	777 778	N	GLN C	101	26.630	26.825	48.185	1.00	145.91
	779	CA CB	GLN C GLN C	101	25.309	26.876	47.562	1.00	145.91
15	780	CG	GLN C	101 101	25.060 24.842	28.258 29.331	46.960	1.00	202.42
	781	CD	GLN C	101	23.913	28.865	47.995 49.091	1.00 1.00	202.42
	782	OE1	GLN C	101	24.266	27.997	49.893	1.00	202.42 202.42
	783	NE2	GLN C	101	22.712	29.428	49.123	1.00	202.42
20	784	C	GLN C	101	25.106	25.805	46.487	1.00	145.91
20	785 786	0 N	GLN C	101	26.031	25.063	46.149	1.00	145.91
	787	CD	PRO C PRO C	102 102	23.886 22.626	25.701	45.939	1.00	126.29
***	788	CA	PRO C	102	23.621	26.310 24.698	46.410	1.00	226.98
	789	СВ	PRO C	102	22.151	24.385	44.908 45.124	1.00 1.00	126.29
25	790	CG	PRO C	102	21.598	25.737	45.443	1.00	226.98 226.98
	791	Ç	PRO C	102	23.911	25.213	43.497	1.00	126.29
	792	0	PRO C	102	23.787	26.412	43.199	1.00	126.29
	793 794	N CA	LEU C	103	24.286	24.291	42.620	1.00	131.06
30	795	CB	LEU C	103 103	24.592 26.086	24.644	41.240	1.00	131.06
	796	ČĠ	LEU C	103	26.385	24.692 25.294	41.058 39.703	1.00 1.00	130.31
	797	CD1	LEU C	103	25.983	26.756	39.788	1.00	130.31 130.31
	798	CD2	LEU C	103	27.857	25.143	39.332	1.00	130.31
35	799	Ç	LEU C	103	24.020	23.658	40.214	1.00	131.06
33	800 801	0 N	LEU C	103	24.265	22.458	40.297	1.00	131.06
	802	CA	PHE C PHE C	104 104	23.267 22.698	24.151	39.239	1.00	115.91
	803	CB	PHE C	104	21.177	23.265 23.174	38.229 38.354	1.00	115.91
	804	ĊĠ	PHE C	104	20.701	22.781	39.706	1.00 1.00	184.63 184.63
40	805	CD1	PHE C	104	20.673	23.704	40.748	1.00	184.63
	806	CD2	PHE C	104	20.284	21.483	39.950	1.00	184.63
	807 808	CE1	PHE C	104	20.232	23.335	42.025	1.00	184.63
:	809	CE2 CZ	PHE C PHE C	104 104	19.841	21.104	41.225	1.00	184.63
45	810	č	PHE C	104	19.815 23.026	22.034 23.754	42.264 36.826	1.00	184.63
	811	ō	PHE C	104	22.731	24.898	36.484	1.00 1.00	115.91
	812	N	LEU C	105	23.636	22.890	36.025	1.00	115.91 135.47
	813	CA	LEU C	105	23.955	23.247	34.643	1.00	135.47
50	814 815	CB	LEU C	105	25.417	23.009	34.331	1.00	111.96
50	816	CG CD1	LEU C	105 105	26.347 27.796	23.800	35.242	1.00	111.96
	817	CD2	LEU C	105	27.796 25.961	23.589 25.269	34.767	1.00	111.96
	818	C	LEU C	105	23.101	22.381	35.233 33.740	1.00	111.96
	819	0	LEU C	105	22.734	21.264	33.740 34.094	1.00 1.00	135.47 135.47
55	820	N	ARG U	106	22.782	22.888	32.564	1.00	142.54
	821 822	CA	ARG C	106	21.928	22.134	31.679	1.00	142.54
	823	CB CG	ARG C	106	20.500	22.619	31.876	1.00	187.32
	824	CD	ARG C ARG C	106 106	19.479	21.927	31.044	1.00	187.32
60	825	NE	ARG C	106	18.129 17.177	22.598 22.007	31.190 30.262	1.00	187.32
	826	CZ	ARG C	106	16.158	22.658	29.719	1.00 1.00	187.32 187.32
	827	NH1	ARG C	106	15.956	23.937	30.020	1.00	187.32
	828	NH2	ARG C	106	15.359	22.032	28.858	1.00	187.32
65	829	C	ARG C	106	22.347	22.297	30.232	1.00	142.54
95	830 831	O N	ARG C CYS C	106	22.485	23.424	29.750	1.00	142.54
	832	GA CA	CYS C	107 107	22.580 22.950	21.177	29.547	1.00	145.66
	833	Č	CYS C	107	21.612	21.221 21.282	28.129 27.439	1.00	145.66
70	834	0	CYS C	107	20.923	20.257	27.459	1.00 1.00	145.66 145.66
70	835	CB	CYS C	107	23.679	19.945	27.717	1.00	147.17
								-	

	836 837	SG N	HIS C	108 2	4.521 1.242	20.003 22.477	26.086 26.975 26.334	1.00 1.00 1.00	147.17 187.51 187.51
	838	CA			9.945	22.697 24.051	26.763	1.00	249.50
	839	CB .		•	9.369 7.934	24.251	26.389	1.00	249.50
5	840	CG	HIS C HIS C		7.311	25.271	25.756	1.00	249.50
	841	CD2	HIS C HIS C		6.945	23.348	26.724	1.00	249.50
	842	ND1 CE1	HIS C		5.777	23.808	26.317	1.00	249.50
	843 844	NE2	HIS C		5.969	24.974	25.727	1.00 1.00	249.50 187.51
10	845	C	HIS C		9.929	22.622	24.824 24.148	1.00	187.51
10	846	0	HIS C		20.677	23.334 21.765	24.310	1.00	207.18
	847	N	GLY C		9.049 8.916	21.601	22.879	1.00	207.18
	848	ÇA	GLY C		17.989	22.668	22.337	1.00	207.18
٠,-	849	C O	GLY C		7.304	23.341	23.106	1.00	207.18
15	850	N	TRP C		17.976	22.837	21.017	1.00	133.19 133.19
	851 852	CA	TRP C		17.119	23.828	20.384 19.044	1.00 1.00	164.64
	853	СВ	TRP C		17.724	24.269	18.221	1.00	164.64
	854	CG	TRP C		16.806	25.128 26.561	18.110	1.00	164.64
20	855	CD2	TRP C		16.829 15.742	26.928	17.286	1.00	164.64
	856	CE2	TRP C		17.659	27.566	18.625	1.00	164.64
	857	CE3 CD1	TRP C		15.753	24.710	17.479	1.00	164.64
	858 eso	NE1	TRP C	110	15.103	25.780	16.917	1.00 1.00	164.64 164.64
25	859 860	CZ2	TRP C	110	15.460	28.261	16.964 18.301	1.00	164.64
23	861	CZ3	TRP C	110	17.380	28.901 29.231	17.474	1.00	164.64
	862	CH2	TRP C	110	16.285	23.243	20.194	1.00	133.19
	863	С	TRP C	110 110	15. 71 1 15. 535	22.018	20.064	1.00	133.19
	864	0	TRP C ARG C	111	14.709	24.124	20.194	1.00	142.65
30	865	N CA	ARG C	111	13.309	23.711	20.051	1.00	142.65 249.69
	866 967	CB	ARG C	111	13.020	23.259	18.618	1.00 1.00	249.69
	867 868	CG	ARG C	111	12.569	24.383	17.699 16.409	1.00	249.69
	869	CD	ARG C	111	11.976	23.832 24.593	16.004	1.00	249.69
35	870	NE	ARG C	111	10. 79 9 9. 704	24.725	16.755	1.00	249.69
	871	CZ	ARG C ARG C	111 111	9.634	24.144	17.952	1.00	249.69
	872	NH1 NH2	ARG C	111	8.674	25.440	16.311	1.00	249.69 142.65
	873 874	C	ARG C	111	12.979	22.588	21.013	1.00 1.00	142.65
40	875	ŏ	ARG C	111	12.125	21.759	20.747 22.137	1.00	230.43
40	876	N	ASN C	112	13.675	22.582 21.574	23.156	1.00	230.43
	877	CA	ASN C	112 112	13.477 12.133	21.797	23.858	1.00	249.69
	878	CB	ASN C ASN C	112	12.030	21.045	25.178	1.00	249.69
4 5	879	CG OD1	ASN C	112	12.829	20.147	25.466	1.00	249.69 249.69
45	880	ND2	ASN C	112	11.036	21.404	25.983	1.00 1.00	230.43
	881 882	C	ASN C	112	13.531	20.163	22.573 23.075	1.00	230.43
	883	Õ	ASN C	112	12.862	19.257 19.970	21.511	1.00	206.47
	884	N	TRP C	440	14.310 14.426	18.637	20.916	1.00	206.47
50		CA	TRP C	113 113	15.220	18.665	19.611	1.00	233.56
	886	CB	TRP C	113	14.430	19.060	18.428	1.00	233.56
	887	CG CD2	TRP C	113	14.905	19.800	17.309	1.00	233.56 233.56
	888 889	CE2	TRP C	113	13.832	19.895	16.392 16.990	1.00 1.00	233.56
55	890	CE3	TRP C	113	16.129	20.395	18.158	1.00	233.56
	891	CD1	TRP C	113	13.132 12.764	18.740 19.239	16.937	1.00	233.56
	892	NE1	TRP C	113 113		20.566	15.166		233.56
	893	CZ2	TRP C	113	16.253	21.061	15.772		233.56
21	894	CZ3 CH2	TRP C	113	15.165	21.139	14.873		233.56 206.47
60) 895 896	C	TRP C	113	15.137	17.714	21.887		206.47
	897	· ŏ	TRP C	113	15.328	18.062	23.050 21.408		249.46
	898	N	ASP C	114		16.540 15.589	22.256		249.46
	899	CA	ASP C	114		14.218	22.229		249.69
6		CB	ASP C	114 114		14.137	23.189	1.00	249.69
	901	CG OD1	ASP C			14.363	24.407		249.69 249.69
	902 903	OD2	ASP C	114	13.227	13.838	22.729		249.46
	903	C	ASP C	: 114		15.447	21.834 20.64		249.46
7	0 905	Ó	ASP C	; 114	18.008	15.291	20.04		
-									

	906 907 908	N CA CB	VAL C VAL C VAL C	115 115 115	18.602 20.027 20.831	15.512 15.388 16.572	22.818 22.545	1.00	150.51 150.51
5	909 910 911	CG1 · CG2 C	VAL C VAL C VAL C	115 115 115	22.243 20.140 20.559	16.592 17.884 14.078	23.147 22.569 22.859 23.135	1.00 1.00 1.00 1.00	133.46 133.46 133.46
10	912 913 914	O N CA	VAL C TYR C TYR C	115 116 116	20.153 21.468 22.066	13.669 13.432 12.170	24.225 22.404 22.826	1.00 1.00 1.00	150.51 150.51 198.57
10	915 916 917	CB CG CD1	TYR C TYR C TYR C	116 116 116	21.673 20.185 19.350	11.070 10.787 11.339	21.847 21.832 20.856	1.00 1.00 1.00	198.57 249.69 249.69 249.69
15	918 919 920 921	CE1 CD2 CE2 CZ	TYR C TYR C TYR C	116 116 116	17.974 19.608 18.241	11.099 9.987 9.741	20.866 22.816 22.838	1.00 1.00 1.00	249.69 249.69 249.69
	922 923 924	ОН С О	TYR C TYR C TYR C TYR C	116 116 116 116	17.429 16.075 23.582 24.174	10.296 10.047 12.257 13.239	21.865 21.894 22.914	1.00 1.00 1.00	249.69 249.69 198.57
20	925 926 927	N CA CB	LYS C LYS C LYS C	117 117 117	24.198 25.660 26.357	11.230 11.186 10.893	22.455 23.500 23.661 22.320	1.00 1.00 1.00 1.00	198.57 159.55 159.55
25	928 929 930	CG CD CE	LYS C LYS C	117 117 117	26.455 27.543 28.915	9.408 9.165 9.642	21.969 20.910 21.399	1.00 1.00 1.00	249.69 249.69 249.69 249.69
	931 932 933 934	NZ C O N	LYS C LYS C LYS C	117 117 117	30.027 26.242 27.200	9.430 12.486 13.081	20.424 24.245 23.698	1.00 1.00 1.00	249.69 159.55 159.55
30	935 936 937	CA CB CG1	VAL C VAL C VAL C VAL C	118 118 118 118	25.675 26.095 24.919 25.416	12.904 14.127 14.737 15.626	25.371 26.016 26.790	1.00 1.00 1.00	141.55 141.55 150.57
35	938 939 940	CG2 C	VAL C VAL C VAL C	118 118 118	24.067 27.305 27.466	15.543 14.028 13.067	27.908 25.830 26.927 27.672	1.00 1.00 1.00 1.00	150.57 150.57 141.55 141.55
	941 942 943	N CA CB	ILE C	119 119 119	28.140 29.358 30.578	15.062 15.192 14.818	26.850 27.640 26.826	1.00 1.00 1.00	119.98 119.98 122.95
40	944 945 946 947	CG2 CG1 CD1 C	ILE C ILE C ILE C	119 119 119	31.814 30.368 31.187	14.861 13.438 13.228	27.700 26.214 24.988	1.00 1.00 1.00	122.95 122.95 122.95
45	948 949 950	O N CA	ILE C TYR C TYR C	119 119 120 120	29.528 29.454 29.744 29.962	16.649 17.518 16.919 18.289	28.029 27.179 29.310 29.759	1.00 1.00 1.00 1.00	119.98 119.98 136.43
	951 952 953	CB CG CD1	TYR C TYR C TYR C	120 120 120	29.334 27.833 27.125	18.542 18.525 17.332	31.119 31.107 31.234	1.00 1.00 1.00	136.43 134.07 134.07 134.07
50	954 955 956	CE1 CD2 CE2	TYR C TYR C TYR C	120 120 120	25.733 27.113 25.721	17.310 19.704 19.705	31.200 30.949 30.912	1.00 1.00 1.00	134.07 134.07 134.07
55	957 958 959 960	CZ OH C O	TYR C TYR C TYR C TYR C	120 120 120	25.037 23.658 31.455	18.507 18.523 18.459	31.037 30.988 29.877	1.00 1.00 1.00	134.07 134.07 136.43
	961 962 963	N CA CB	TYR C TYR C TYR C	120 121 121 121	32.171 31.935 33.366 33.991	17.497 19.674 19.916 20.177	30.131 29.682 29.782 28.405	1.00 1.00 1.00 1.00	136.43 132.15 132.15
60	964 965 966	CG CD1 CE1	TYR C TYR C TYR C	121 121 121	34.032 32.863 32.889	19.017 18.383 17.388	27.437 27.007 26.038	1.00 1.00 1.00	142.37 142.37 142.37 142.37
65	967 968 969	CD2 CE2 CZ	TYR C TYR C TYR C	121 121 121	35.237 35.284 34.098	18.620 17.616 17.005	26.879 25.900 25.481	1.00 1.00 1.00	142.37 142.37 142.37
UJ	970 971 972 973	о С ОН	TYR C TYR C TYR C LYS C	121 121 121	34.141 33.668 33.025	16.024 21.119 22.159	24.499 30.667 30.543	1.00 1.00 1.00	142.37 132.15 132.15
70	974 975	CA CB	LYS C	122 122 122	34.650 35.056 34.793	20.977 22.076 21.754	31.554 32.413 33.878	1.00 1.00 1.00	126.92 126.92 206.28

				05 477	22,888	34.807	1.00	206.28
	976	CG		122 35.177 122 35.209	22.420	36.238	1.00	206.28
	977	CD		122 35.209 122 35.768	23,480		1.00	206.28
	978	CE		122 35.923	22.930	38.515	1.00	206.28
_	979	NZ	LYS C	122 36.544	22,299	32.193	1.00	126.92 126.92
5	980	C O		122 37.349	21.420	32.461	1.00 1.00	135.65
	981	N	ASP C	123 36.902	23.477	31.699 31.435	1.00	135.65
	982 983	CA	ASP C	123 38.294	23.827	32,740	1.00	170.94
	984	CB	ASP C	123 39.093	23.949 25.212	33.507	1.00	170.94
10	985	CG	ASP C	123 38.763 123 38.780	26.308	32.904	1.00	170.94
••	986	OD1	ASP C	123 38.780 123 38.496	25.117	34.721	1.00	170.94
	987	OD2	ASP C	123 38.987	22.847	30.509	1.00	135.65
	988	CO	ASP C	123 40.082	22.372	30.818	1.00 1.00	135.65 178.68
15	989 990	N	GLY C	124 38.345	22.547	29.378 28.395	1.00	178.68
13	991	CA	GLY C	124 38.917	21.638	28.718	1.00	178.68
	992	C	GLY C	124 38.936	20.152 19.336	27.879	1.00	178.68
	993	0	GLY C	124 39.295 125 38.539	19.797	29.929	1.00	128.18
	994	N	GLU C	125 38.539 125 38.536	18.407	30.368	1.00	128.18
20	995	CA	GLU C	125 38.963	18.324	31.847	1.00	249.69
	996	CB CG	GLU C	125 40.422	18.660	32.115	1.00 1.00	249.69 249.69
	997	CD	GLU C	125 41.355	17.552	31.693 32.273	1.00	249.69
	998 999	OE1	GLU C	125 41.251		30.786	1.00	249.69
25	1000	OE2	GLU C	125 42.189		30.215	1.00	128.18
20	1001	С	GLU C	125 37.176 125 36.149		30.403	1.00	128.18
	1002	0	GLU C	125 36.149 126 37.165		29.866	1.00	114.67
	1003	N	ALA C ALA C	126 35.904	4-740	29.753	1.00	114.67
	1004	CA	ALA C ALA C	126 36.156	14.376	29.162	1.00	125.78 114.67
30	1005	CB C	ALA C	126 35.39	7 15.622	31.195 32.099	1.00 1.00	114.67
	1006 1007	ŏ	ALA C	126 36.19		31.437	1.00	136.95
	1008	N	LEU C	127 34.10		32.816	1.00	136.95
	1009	CA	LEU C	127 33.63 127 33.09		33.235	1.00	112.43
35	1010	CB	LEU C	127 33.09 127 33.25		34.734	1.00	112.43
	1011	CG	LEU C	127 34.72	5 17.020	35.093	1.00	112.43 112.43
	1012	CD1 CD2	LEU C	127 32.76	8 18.588	35.170	1.00 1.00	136.95
	1013 1014	C	LEU C	127 32.61		33.156 34.019	1.00	136.95
40	1015	ŏ	LEU C	127 32.87		32.518	1.00	111.10
40	1016	N	LYS C	128 31.44	' '	32.750	1.00	111.10
	1017	CA	LYS C	128 30.39 128 29.23		33.525	1.00	196.03
	1018	CB	LYS C	128 29.5		34.905	1.00	196.03 196.03
4.6	1019	CD	LYS C	128 29.8	64 13.714	35.892	1.00 1.00	196.03
45	5 1020 1021	CE	LYS C	128 30.1		37.285 38.329	1.00	196.03
	1022	NZ	LYS C	128 30.1		31.379	1.00	111.10
	1023	C	L'IS C	128 29.9		30.360	1.00	111.10
	1024	0	LYS C	128 30.1 129 29.2		31.339	1.00	147.54
50	0 1025	N.	TYR C	129 29.2 129 28.7		30.058	1.00	147.54
	1026	CA	TYR C	129 29.8		29.363	1.00	149.35 149.35
	1027	CB CG	TYR C	129 29.2	282 9.856	28.292	1.00 1.00	149.35
	1028 1029	CD1	TYR C	129 29.0		27.005 26.029	1.00	149.35
5	5 1030	CE1	TYR C	129 28.		28.584	1.00	149.35
	1031	CD2	ITH C	129 28.1 129 28.1		27.619	1.00	149.35
	1032	CE2	TYR C	129 28.1 129 28.		26.340	1.00	149.35
	1033	CZ	TYR C TYR C		613 7.363	25.373		149.35 147.54
,	1034	ОH	TYR C		500 10.704	30.177		147.54
C	50 1035 1036	C	TYR C	129 27.	384 9.893	31.098		199.38
	1036	Ň	TRP C		571 10.876	29.231 29.216		199.38
	1038	CA	TRP C	130 25	323 10.109 219 10.809	30.022		218.46
	1039	CB	TRP C		.219 10.809 .599 11.335	31.370	1.00	218.46
(55 1040	CG	TRP C		.246 10.782	32.632	1.00	218.46
	1041	CD2	TRP C		.770 11.627	33.631		218.46 218.46
	1042	CE2 CE3	TRP C	130 23	.517 9.648	33.029		218.46
	1043 1044	CD1	TRP C	130 25	12.465			218.46
	70 1045	NE1	TRP C	; 130 25	5.431 12.652	J00	•	

	1046	CZ2	11.0		4.605 3.349	11.381 9.398	34.996 34.390	1.00 1.00	218.46 218.46
	1047	CZ3			3.895	10.258	35.357	1.00	218.46
	1048	CH2	,		3.003 4.794	9.910	27.794	1.00	199.38
_	1049	Ç			5.272	10.526	26.839	1.00	199.38
5	1050	0	1110 -		23.787	9.053	27.671	1.00	229.56 229.56
	1051	N CA	TYR C		23.148	8.778	26.386	1.00 1.00	246.37
	1052	CA CB	TYR C	131	22.591	7.356	26.372 24.998	1.00	246.37
	1053	CG	TYR C		22.180	6.894	24.990	1.00	246.37
10	1054 1055	CD1	TYR C		23.142	6.593	22.748	1.00	246.37
10	1056	CE1	TYR C		22.771	6.206 6.795	24.647	1.00	246.37
	1057	CD2	TYR C		20.834 20.454	6.411	23.370	1.00	246.37
	1058	CE2	TYR C		20.45 4 21.422	6.120	22.425	1.00	246.37
	1059	CZ	TYR C		21.422	5.759	21.152	1.00	246.37
15	1060	он	TYR C TYR C		22.003	9.783	26.290	1.00	229.56 229.56
	1061	C	TYR C	131	22.194	10.887	25.767	1.00	249.69
	1062	0 N	GLU C	132	20.814	9.387	26.766	1.00 1.00	249.69
	1063	CA	GLU C	132	19.674	10.303	26.812 27.444	1.00	249.69
20	1064	CB	GLU C	132	18.455	9.632	26.529	1.00	249.69
20	1065 1066	ČĞ	GLU C	132	17.670	8.696 9.186	26.293	1.00	249.69
	1067	CD	GLU C	132	16.251	10.108	27.021	1.00	249.69
	1068	OE1	GLU C	132	15.815	8.651	25.388	1.00	249.69
	1069	OE2	GLU C	132 132	15.566 20.299	11.278	27.798	1.00	249.69
25	1070	С	GLU C	132	20.255	10.849	28.865	1.00	249.69
	1071	0	GLU C ASN C	133	20.318	12.573	27.483	1.00	172.36 172.36
	1072	N	ASN C	133	21.034	13.476	28.374	1.00 1.00	175.23
	1073	CA	ASN C	133	21.319	14.844	27.675	1.00	175.23
	1074	CB CG	ASN C	133	20.166	15.840	27.735 27.529	1.00	175.23
30	1075	OD1	ASN C	133	18.999	15.492	27.974	1.00	175.23
	1076 1077	ND2	ASN C	133	20.506	17.113 13.626	29.815	1.00	172.36
	1078	C	ASN C	133	20.565	12.906	30.290	1.00	172.36
	1079	0	ASN C	133	19.680 21. 23 8	14.521	30.522	1.00	165.75
35	1080	N	HIS C	134 134	20.960	14.757	31.918	1.00	165.75
•	1081	CA	HIS C HIS C	134	21.912	13.910	32.756	1.00	249.69 249.69
	1082	CB	HIS C HIS C	134	21.588	13.916	34.223	1.00 1.00	249.69
	1083	CG CD2	HIS C	134	22.305	14.372	35.277 34.715	1.00	249.69
40	1084	ND1	HIS C	134	20.407	13.441	36.041	1.00	249.69
40	1085 1086	CE1	HIS C	134	20.390	13.599	36.397	1.00	249.69
	1087	NE2	HIS C	134	21.526	14.161 16.233	32.200	1.00	165.75
	1088	С	HIS C	134	21.166	17.050	31.285	1.00	165.75
	1089	0	HIS C	134	21. 223 21. 27 8	16.572	33.470	1.00	159.28
45	1090	N	ASN C	135 135	21.467	17.948	33.879	1.00	159.28 249.51
	1091	CA	ASN C ASN C	135	20.111	18.596	34.178	1.00	249.51
	1092	CB	ASN C	135	19.266	18.779	32.923	1.00 1.00	249.51
	1093	CG OD1	ASN C	135	19.783	19.248	31.903 32.990	1.00	249.51
51	1094	ND2	ASN C	135		18.439	35.116	1.00	159.28
50) 1095 1096	C	ASN C	135		18.001 18.086	36.253		159.28
	1097	ŏ	ASN C	135		17.946	34.884		134.89
	1098	N	ILE C	138		17.989	35.934		134.89
	1099	CA	ILE C	136		18.399	35.318		169.29
5	5 1100	CB	ILE C	136 136		19.723	34.593		169.29 169.29
_	1101	CG2	ILE C			18.510	36.407		169.29
	1102	CG1	ILE C			18. 98 0	35.884		134.89
	1103	CD1	ILE C			18.906	37.123		134.89
	1104	C	ILE C		6 24.498	20.125	37.049 38.23		137.39
C	1105	Ň	SER C	; 13		18.280	39.42		137.39
	1106 1107	ČA	SER C	; 13		19.000 18.437	39.94	0 1.00	121.23
	1107	СВ	SER	; 13		18.966	41.22	2 1.00	121.23
	1109	OG	SER C	13		19.025	40.56	6 1.00	137.39
(65 1110	Ç	SER C) 13 3 13		18.081	40.77		137.39
`	1111	0	SER		38 24.647	20.113	41.33		121.18 121.18
	1112	N			38 25.539	20.309	42.47		97.12
	1113	CA CB			38 26.683	21.238	42.10		97.12
	70 4445	CG2	:: <u> </u>		38 27.385	21.749	43.35	00.00	
	70 1115		-		•	•			

•							41.187	1.00	97.12
			ILE C	138	27.646	20.502	40.528	1.00	97.12
1	116	~ .	ILE C ILE C	138	28.637	21.411 20.886	43.697	1.00	121.18
•	1117	001	ILE C	138	24.814	20.866 21.966	43.651	1.00	121.18
	1118		ILE C	138	24,212	20.145	44.796	1.00	175.86 175.86
_	1119	N	THR C	139	24.890 24.253	20.532	46.042	1.00 1.00	224.21
	1120 1121	CA	THR C	139 139	24.065	19.297	46,929 47.063	1.00	224.21
	1122	CB	THR C	139	25.324	18.622	46.298	1.00	224.21
	1123	OG1	THR C	139	23.061	18.341 21.539	46.745	1.00	175.86
	1124	CG2	THR C	139	25.144	21.535	46.654	1.00	175.86 196.19
10	1125	C	THR C	139	24.927	21.024	47.447	1.00	196.19
	1126	N	ASN C	140	26.149 27.111	21.852	48.165	1.00 1.00	249.69
	1127 1128	CA	ASN C	140 140	27.710	21.053	49.330 50.109	1.00	249.69
	1129	CB	ASN C	140	28.741	21.837	49.523	1.00	249.69
15	1130	CG	ASN C	140	29.656	22.417	51.432	1.00	249.69
15	1131	OD1	ASN C	140	28.610	21.845 22.213	47.146	1.00	196.19
	1132	ND2 C	ASN C	140	28.184	21.327	46.560	1.00	196.19 134.37
	1133	Ö	ASN C	140	28.799 28.400	23.507	46.932	1.00 1.00	134.37
20	1134 1135	Ň	ALA C	141	29.383	23.954	45.949	1.00	79.03
20	1136	CA	ALA C	141 141	28.834	25.131	45.148 46.507	1.00	134.37
	1137	CB	ALA C ALA C	141		24.317	47,452	1.00	134.37
	1138	C	ALA C	141	30.896	25.112 23.724	45.898	1.00	119.18
_	1139	0	THR C	142		23.954	46.281	1.00	119.18 209.05
25	1140	N CA	THR C	142		22,720	46.002	1.00	209.05
	1141	CB	THR C	142		21.553	46.578	1.00 1.00	209.05
	1142 1143	0G1	THR C	14: 14:		22.907	46.602 45.416	4.00	119.18
	1144	CG2	THR C	14		25.093	44.356		119.18
30		C	THR C	14	2 33.128	25.381 25.741	45.865	1.00	145.21
•	1146	0	VAL C	14		26.836	45.096	1.00	145.21 137.97
	1147	N GA	VAL C			27.672	45.910		137.97
	1148 1149	CB	VAL C			26.915	46.09		137.97
35		CG1	VAL C		43 37.596 43 36.549	28.993	45.20 43.87		145.21
J.	1151	CG2	VAL C		43 36.023	26.287	42.88	1.00	145.21
	1152	C	VAL	•	43 36.183		43.95	6 1.00	198.77 198.77
	1153	0 N	GLU	3 1	44 36.469	20.445	42.83		249.69
4	1154	CA	GLU (3 1	44 37.176	50 140	43.24		249.69
4	() 1155 1156	CB	GLU	_	144 37.856 144 38.885	; 23.312	44.33 45.63		249.69
	1157	CG	GLU GLU	_	144 38.44	7 22.661	45.6 45.6		249.69
	1158	CD	GLU		144 38.25		46.6	39 1.00	249.69
	1159	OE1	GLU	č	144 38.29	- 470	41.6	94 1.00	
4	5 1160	OE2 C	GLU	С	144 36.21 144 36.65	-0.000	40.5		400 E1
	1161	ŏ	GLU	С		24.274	41.9		400 51
	1162 1163	Ň	ASP	C	145 34.91 145 33.90	u 24.049	40.9 41.) 171.03
	1164	CA	ASP ASP	C	145 32.5	23.868		138 1.00	171.03
:	50 1165	СВ	ASP	Č	145 32.3			380 1.00	
	1166	CG OD1			145 32.4		40	.340 1.0	400 E4
	1167	OD2	ASP	C	145 32.0 145 33.8	013	39	.939 1.0	400.01
	1168 1169	_	ASP	C	170	~ ~ ~ ~ ~ ~	38	.851 1.0	
	55 1170	_	ASF	C	145 34.4 146 34.4	161 26.342		.327 1.0 .491 1.0	0 126.39
	1171	N	200	3 C	146 34.	505 27.546	,	270 1.0	00 126.60
	1172	CA		àC	146 35.		•	1.449 1.0	
	1173		-	R C	,	77 30	1 3	,,,,,	
	1174	•	SE	RÇ		343 27.30 478 26.85	ი 3	J.00 .	00 126.39 00 222.43
	60 117	_	SE	RC		. 798 27.6 1	~		00 222.43
	117	7 N	-	Y C		550 27.41			.00 222.43
	117	'8 C/	` ~	Y C	147 34	.769 27.77	20 3	4.682 1	.00 222.43
	117	rg C	GI	Y C	147 33	.801 28.53 187 27.23	36	33.463	.00 ACO OF
	65 116		Th	IR C		07 E	06 3	32.186 ¹	,00
	110	,,	A TI	4R C		474 28.2	53	J (,== 0 ·	1.00 134.31 1.00 134.31
	110	83 C	8 <u>Ti</u>	HR C		6.046 27.3	20		1.00 134.31
	11	84 C	_	HR C		8.609 28.9	43	31.810	
		85 C	G2 T	nn O					

1191										
1188		4400	_	TUD C	140	33 040	26 223	31.538	1.00	128.05
1188					-					128.05
1189 CA										106.87
5 1190 CB TYR C 149 30.819 24.510 31.905 1.00 1191 CB TYR C 149 31.204 24.226 33.336 1.00 1192 CD1 TYR C 149 31.204 24.226 33.336 1.00 1193 CB1 TYR C 149 31.204 22.554 34.210 1.00 1193 CB1 TYR C 149 31.247 22.922 33.816 1.00 1194 CD2 TYR C 149 31.247 22.922 33.816 1.00 1195 CB TYR C 149 31.247 22.922 33.816 1.00 1195 CB TYR C 149 31.247 22.922 33.816 1.00 1195 CB TYR C 149 31.247 22.922 33.816 1.00 1195 CB TYR C 149 31.247 22.922 33.816 1.00 1195 CB TYR C 149 31.228 23.676 35.993 1.00 1198 CB TYR C 149 31.228 23.676 35.993 1.00 1198 CB TYR C 149 31.208 23.676 35.993 1.00 1198 CB TYR C 149 31.208 23.676 35.993 1.00 1198 CB TYR C 149 31.208 23.676 35.993 1.00 1198 CB TYR C 150 31.00 29.567 1.00 1200 CB TYR C 150 31.00 29.567 1.00 1200 CB TYR C 150 31.00 23.953 28.946 1.00 1200 CB TYR C 150 31.451 24.907 26.499 1.00 1200 CB TYR C 150 31.451 24.907 26.499 1.00 1200 CB TYR C 150 32.201 22.195 25.317 1.00 1200 CB TYR C 150 33.199 21.307 26.499 1.00 1200 CB TYR C 150 33.873 21.307 26.499 1.00 1200 CB TYR C 150 33.873 21.307 26.591 1.00 1200 CB TYR C 150 33.873 21.307 26.591 1.00 1200 CB TYR C 150 33.873 21.576 26.551 1.00 1200 CB TYR C 150 33.873 21.507 24.672 1.00 1200 CB TYR C 150 33.873 21.507 24.672 1.00 1200 CB TYR C 150 33.853 21.594 25.519 1.00 1200 CB TYR C 150 33.853 21.594 25.519 1.00 1201 CB TYR C 150 33.853 21.594 25.519 1.00 1201 CB TYR C 150 33.853 21.594 25.519 1.00 1201 CB TYR C 150 33.507 20.693 24.719 1.00 1201 CB TYR C 150 33.507 20.693 24.719 1.00 1201 CB TYR C 150 33.507 20.693 24.719 1.00 1201 CB TYR C 150 33.507 20.693 24.719 1.00 1201 CB TYR C 150 33.507 20.693 24.719 1.00 1201 CB TYR C 150 33.507 12.507 20.693 24.719 1.00 1201 CB TYR C 150 33.507 12.507 24.692 1.00 1201 CB TYR C 150 30.707 24.692 1.00 1										106.87
1191	5			TYR C					1.00	100.05
1192	5							33.336	1.00	100.05
1193							25.254	34.210	1.00	100.05
1194						31.799	24.992	35.538	1.00	100.05
10			CD2	TYR C	149	31.247			1.00	100.05
1187	10		CE2	TYR C	149					100.05
1198		1196								100.05
1199 O TYR C 149 31.228 26.210 29.077 1.00 1201 CA TYR C 150 31.105 23.953 28.948 1.00 1202 CB TYR C 150 31.405 23.953 28.948 1.00 1203 CG TYR C 150 31.451 24.307 26.499 1.00 1203 CG TYR C 150 32.201 22.195 25.317 1.00 1204 CD1 TYR C 150 32.201 22.195 25.317 1.00 1205 CE1 TYR C 150 32.201 22.195 25.317 1.00 1206 CD2 TYR C 150 33.199 21.307 24.872 1.00 1207 CE2 TYR C 150 33.199 21.307 24.872 1.00 1208 CZ TYR C 150 33.873 23.576 26.351 1.00 1209 CH TYR C 150 34.830 22.598 25.912 1.00 1209 CH TYR C 150 34.830 22.598 25.912 1.00 1209 CH TYR C 150 34.533 21.564 25.169 1.00 1211 O TYR C 150 30.700 21.521 28.119 1.00 1212 N CYS C 151 28.711 20.094 26.450 1.00 1214 C CYS C 151 28.711 20.094 26.450 1.00 1214 C CYS C 151 28.660 20.289 24.796 1.00 1216 CB CYS C 151 28.660 20.289 24.796 1.00 1217 SQ CYS C 151 28.660 20.289 24.796 1.00 1218 N THR C 152 28.660 20.289 24.796 1.00 1219 CA THR C 152 28.675 18.446 23.358 1.00 1218 N THR C 152 28.671 18.981 24.715 1.00 1219 CA THR C 152 30.004 17.832 22.911 10.00 1218 N THR C 152 28.671 18.981 24.715 1.00 1221 OG1 THR C 152 30.004 17.838 22.951 1.00 1222 CG2 THR C 152 31.182 18.762 23.354 1.00 1223 CG THR C 152 30.004 17.838 22.951 1.00 1224 O THR C 152 30.004 17.838 22.951 1.00 1225 N GLY C 153 25.800 16.180 21.992 1.00 1226 CA THR C 152 27.620 11.6582 23.354 1.00 1227 C GLY C 153 25.980 16.180 21.992 1.00 1228 N GLY C 153 25.980 16.180 21.992 1.00 1229 N GLY C 153 25.980 16.180 21.992 1.00 1229 N GLY C 153 25.980 16.180 21.992 1.00 1238 N VAL C 153 25.980 16.180 21.992 1.00 1239 CA THR C 152 27.631 17.343 23.278 1.00 1226 CG THR C 152 27.631 17.343 23.278 1.00 1227 C GLY C 153 25.980 16.180 21.992 1.00 1228 C G HR C 152 27.631 17.343 23.278 1.00 1229 N GLY C 153 25.980 16.180 21.992 1.00 1236 C THR C 152 27.400 16.609 24.240 1.00 1236 C THR C 152 27.400 16.609 24.240 1.00 1236 C THR C 152 27.400 16.609 24.240 1.00 1236 C THR C 155 21.397 15.780 17.797 1.00 1238 N VAL C 155 21.397 15.780 17.797 1.00 1239 CA VAL C 155 21.397 15.780 17.797 1.00 1230 CA VAL C 155 21.397 15.780 17.7		1197								100.05
15 1200 N TYR C 150 31.105 23.953 28.946 1.00 1201 CA TYR C 150 30.490 23.838 27.614 1.00 1202 CB TYR C 150 30.490 23.838 27.614 1.00 1203 CG TYR C 150 31.451 24.307 26.499 1.00 1204 CD1 TYR C 150 32.523 23.336 26.058 1.00 1206 CD2 TYR C 150 33.199 21.307 24.872 1.00 1206 CD2 TYR C 150 33.199 21.307 24.872 1.00 1207 CE2 TYR C 150 33.199 21.307 24.872 1.00 1208 CZ TYR C 150 34.880 22.698 25.912 1.00 1209 CH TYR C 150 34.880 22.698 25.912 1.00 1209 CH TYR C 150 34.853 21.564 25.169 1.00 1209 CH TYR C 150 30.700 21.521 28.119 1.00 1210 C TYR C 150 30.111 22.370 27.462 1.00 1211 O TYR C 150 30.700 21.521 28.119 1.00 1212 N CYS C 151 28.711 20.694 26.450 1.00 1213 CA CYS C 151 28.711 20.694 26.450 1.00 1214 C CYS C 151 28.680 20.293 24.976 1.00 1215 O CYS C 151 28.680 20.293 24.976 1.00 1216 CB CYS C 151 27.359 20.425 27.067 1.00 1217 SG CYS C 151 27.359 20.425 27.067 1.00 1218 N THR C 152 28.711 18.981 24.715 1.00 1219 CA THR C 152 30.034 17.838 22.951 1.00 1219 CA THR C 152 30.034 17.838 22.951 1.00 1221 OG1 THR C 152 30.034 17.838 22.951 1.00 1222 CG2 THR C 152 30.213 16.660 24.240 1.00 1223 C THR C 152 30.213 16.660 24.240 1.00 1224 O THR C 152 28.751 18.981 24.715 1.00 1225 N GLY C 153 25.985 17.213 22.122 20.04 1.00 1226 CA GLY C 153 25.985 17.213 22.125 1.00 1227 C GHR THR C 152 20.711 18.981 24.715 1.00 1228 C GA GLY C 153 25.985 17.213 22.125 1.00 1229 C GA GLY C 153 25.985 17.213 22.125 1.00 1220 C GR THR C 152 30.213 16.660 24.240 1.00 1225 N GLY C 153 25.985 17.213 22.125 1.00 1226 CA GLY C 153 25.985 11.597 20.558 1.00 1227 C G GLY C 153 25.985 17.213 22.125 1.00 1228 C G GLY C 153 25.985 17.213 19.10 1229 C G GLY C 153 25.985 11.590 11.7343 22.125 1.00 1224 C G GLY C 153 25.985 17.213 19.10 19.599 1.00 1225 C G GLY C 153 25.985 17.213 19.10 19.599 1.00 1226 C A GLY C 153 25.985 11.590 11.7343 22.125 1.00 1227 C G GLY C 155 21.380 11.7277 11.00 1228 C G LYS C 154 24.240 9.317 15.459 1.00 1229 C G LYS C 154 24.240 9.317 15.459 1.00 1229 C G LYS C 154 24.240 9.317 15.459 1.00 1224 C G LYS C 154 24.240 9.3										106.87
1201 CA TYR C 150 30.460 23.838 27.614 1.00 1202 CB TYR C 150 31.451 24.307 26.469 1.00 1203 CG TYR C 150 32.201 22.195 25.317 1.00 1204 CD1 TYR C 150 32.201 22.195 25.317 1.00 1205 CE1 TYR C 150 32.201 22.195 25.317 1.00 1206 CD2 TYR C 150 33.199 21.307 24.872 1.00 1207 CE2 TYR C 150 33.873 23.576 26.351 1.00 1208 CZ TYR C 150 34.830 22.598 25.912 1.00 1209 OH TYR C 150 35.507 20.693 24.719 1.00 1209 OH TYR C 150 35.507 20.693 24.719 1.00 1211 O TYR C 150 30.111 22.370 27.462 1.00 1212 N CYS C 151 29.112 22.074 26.641 1.00 1212 N CYS C 151 28.600 20.283 24.79 1.00 1214 C CYS C 151 28.660 20.283 24.79 1.00 1216 CB CYS C 151 28.660 20.283 24.79 1.00 1217 SG CYS C 151 28.660 20.283 24.79 1.00 1218 N THR C 152 28.671 18.841 24.103 1.00 1218 N THR C 152 28.671 18.844 23.558 1.00 1218 N THR C 152 28.671 18.844 23.558 1.00 1218 N THR C 152 28.671 18.844 23.358 1.00 1218 N THR C 152 28.671 18.844 23.358 1.00 1219 CA THR C 152 30.034 17.838 22.951 1.00 1221 OG1 THR C 152 30.213 16.582 23.614 1.00 1222 CG2 THR C 152 30.2034 17.838 22.951 1.00 1223 C THR C 152 30.2034 17.838 22.951 1.00 1224 O THR C 152 28.675 18.446 23.358 1.00 1225 N GLY C 151 25.980 16.800 24.240 1.00 1226 CA GLY C 153 25.980 16.800 24.240 1.00 1227 C GLY C 153 25.980 16.800 24.240 1.00 1228 CA LYS C 154 24.249 14.582 19.02 1229 N LYS C 154 24.591 18.981 77.273 1.00 1226 CA LYS C 154 24.249 14.582 19.02 1227 C GLY C 153 25.980 16.180 21.982 1.00 1228 CG LYS C 154 24.590 16.600 24.240 1.00 1228 CG LYS C 154 24.590 16.600 24.240 1.00 1228 N VLS C 154 24.590 16.600 24.240 1.00 1228 CG LYS C 154 24.590 16.600 24.240 1.00 1224 CE LYS C 154 24.590 16.600 9.317 15.459 1.00 1224 CG LYS C 156 19.036 16.800 19.379 1.00 1236 C LYS C 154 24.590 16.600 9.317 15.459 1.00 1237 C GLY C 153 25.980 16.180 17.727 17.00 1238 N VAL C 155 21.397 14.901 19.599 1.00 1239 C A LYS C 154 24.590 16.600 9.317 15.459 1.00 1236 C LYS C 154 24.590 15.575 18.990 1.00 1237 C GLY C 156 19.506 19.508 17.727 17.503 1.00 1238 N VAL C 155 19.500 16.600 9.317 15.459 1.00 1244 C B THR C 156	1.5									106.87 107.82
1202 CB	15									107.82
1204 CD1										160.56
1204									1.00	160.56
20									1.00	160.56
1206	20								1.00	160.56
1207 CE2	20							26.351	1.00	160.56
1208 CZ						34.880	22.698	25.912	1.00	160.56
1209			CZ	TYR C	150	34.533			1.00	160.56
1211			OH		150					160.56
1212	25	1210								107.82
1213										107.82 88.46
1214 C				CYS C						88.46 88.46
1215										88.46
1216 CB CYS C 151 27.359 20.425 27.087 1.00 1217 SG CYS C 151 25.995 21.380 26.5366 1.00 1218 N THR C 152 28.675 18.446 23.358 1.00 1219 CA THR C 152 30.034 17.838 22.951 1.00 1221 OG1 THR C 152 30.034 17.838 22.951 1.00 1221 OG1 THR C 152 30.034 17.838 22.951 1.00 1221 OG1 THR C 152 30.213 16.582 23.614 1.00 1222 CG2 THR C 152 31.182 18.762 23.334 1.00 1224 O THR C 152 27.631 17.343 23.278 1.00 1224 O THR C 152 27.420 16.609 24.240 1.00 1225 N GLY C 153 26.988 17.213 22.125 1.00 1226 CA GLY C 153 25.990 16.180 21.982 1.00 1227 C GLY C 153 25.990 16.180 21.982 1.00 1228 O GLY C 153 25.830 16.783 19.670 1.00 1229 N LYS C 154 24.759 14.905 20.345 1.00 1229 N LYS C 154 24.299 14.582 19.022 1.00 1231 CB LYS C 154 24.531 13.110 18.710 1.0 1232 CG LYS C 154 24.531 13.110 18.710 1.0 1233 CD LYS C 154 24.540 11.227 17.071 1.0 1234 CE LYS C 154 24.540 11.227 17.071 1.0 1236 C LYS C 154 24.400 9.317 15.692 1.0 1237 O LYS C 154 24.400 9.317 15.692 1.0 1238 N VAL C 155 22.748 14.876 18.895 1.0 1239 CA VAL C 155 22.410 15.798 17.793 1.0 1239 CA VAL C 155 22.410 15.798 17.793 1.0 1239 CA VAL C 155 20.918 17.729 17.614 1.0 1244 CG1 VAL C 155 20.918 17.729 17.614 1.0 1246 CA TRP C 156 19.108 17.729 17.614 1.0 1247 CB TRP C 156 19.108 14.172 15.113 1.0 1248 CG C VAL C 155 21.336 18.369 18.918 1.0 1249 CD2 TRP C 156 19.108 14.172 15.113 1.0 1240 CB TRP C 156 19.108 14.172 15.113 1.0 1241 CB1 VAL C 155 21.387 15.758 15.410 1.0 1242 CG2 VAL C 155 21.397 15.758 15.410 1.0 1244 C VAL C 155 21.397 15.758 15.410 1.0 1245 CG2 TRP C 156 19.108 14.172 15.113 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.108 14.172 15.113 1.0 1251 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE2 TRP C 156 15.705 14.788 13.785 1.0 1253 NEI TRP C 156 18.077 17.523 14.010 1.0 1254 CZ2 TRP C 156 15.705 14.788 13.785 1.0	20									88.46
1217 SG CYS C 151 25.995 21.380 26.366 1.00 1218 N THR C 152 28.711 18.981 24.715 1.00 1219 CA THR C 152 28.675 18.446 23.358 1.00 135 1220 CB THR C 152 30.034 17.838 22.951 1.00 1221 OG1 THR C 152 30.213 16.582 23.354 1.00 1222 CG2 THR C 152 37.831 18.762 23.334 1.00 1222 CG2 THR C 152 27.631 17.343 23.278 1.00 1223 C THR C 152 27.631 17.343 23.278 1.00 1224 O THR C 152 27.631 17.343 23.278 1.00 1225 N GLY C 153 26.988 17.213 22.125 1.00 1226 CA GLY C 153 25.980 16.180 21.982 1.00 1227 C GLY C 153 25.980 16.180 21.982 1.00 1228 O GLY C 153 25.980 16.783 19.670 1.00 1229 N LYS C 154 24.759 14.905 20.345 1.00 1231 CB LYS C 154 24.249 14.582 19.0558 1.00 1231 CB LYS C 154 24.249 14.582 19.05 20.345 1.00 1232 CG LYS C 154 24.249 14.582 19.05 20.345 1.00 1233 CD LYS C 154 24.159 12.677 17.303 1.00 1234 CE LYS C 154 24.166 10.749 15.692 1.00 1235 NZ LYS C 154 24.460 9.317 15.459 1.00 1236 C LYS C 154 24.460 9.317 15.459 1.00 1237 O LYS C 154 24.460 9.317 15.459 1.00 1238 N VAL C 155 22.748 14.876 18.895 1.00 1239 CA VAL C 155 22.410 15.798 17.993 1.00 1239 CA VAL C 155 22.410 15.798 17.993 1.00 1239 CA VAL C 155 20.918 17.729 17.614 1.00 1244 CG VAL C 155 20.918 17.729 17.614 1.00 1240 CB VAL C 155 21.336 18.369 18.918 17.727 17.993 1.00 1241 CG1 VAL C 155 20.918 17.729 17.614 1.00 1244 C C C S VAL C 155 20.918 17.729 17.614 1.00 1244 C C C S VAL C 155 20.918 17.729 17.614 1.00 1245 C C S VAL C 155 20.918 17.729 17.614 1.00 1246 CA TRP C 156 19.103 15.124 13.997 1.00 1247 CB TRP C 156 19.103 15.124 13.997 1.00 1248 CG TRP C 156 19.103 15.124 13.997 1.00 1248 CG TRP C 156 19.103 15.124 13.997 1.00 1249 CD2 TRP C 156 15.000 15.936 13.835 1.00 1251 CE3 TRP C 156 15.000 15.936 13.835 1.00 1252 CD1 TRP C 156 16.500 15.936 13.835 1.00 1253 NE1 TRP C 156 18.077 17.523 14.010 1.00 1254 CZ TRP C 156 18.077 17.523 14.010 1.00 1254 CZ TRP C 156 18.077 17.523 14.010 1.00 1254 CZ TRP C 156 18.077 17.523 14.010 1.00	30			CVS C					1.00	149.34
1218 N THR C 152 28.711 18.981 24.715 1.00 1219 CA THR C 152 28.675 18.446 23.358 1.00 35 1220 CB THR C 152 30.034 17.838 22.951 1.00 1221 OG1 THR C 152 30.233 16.582 23.614 1.01 1222 CG2 THR C 152 31.182 18.762 23.334 1.00 1223 C THR C 152 27.631 17.343 23.278 1.00 1224 O THR C 152 27.420 16.609 24.240 1.00 1225 N GLY C 153 26.988 17.213 22.125 1.00 1226 CA GLY C 153 25.980 16.180 21.982 1.00 1227 C GLY C 153 25.980 16.180 21.982 1.00 1228 O GLY C 153 25.880 16.180 21.982 1.00 1229 N LYS C 154 24.759 14.905 20.345 1.00 1229 N LYS C 154 24.249 14.582 19.022 1.00 1231 CB LYS C 154 24.540 11.227 17.071 1.00 1232 CG LYS C 154 24.540 11.227 17.071 1.00 1233 CD LYS C 154 24.460 9.317 15.459 1.00 1234 CE LYS C 154 24.460 9.317 15.459 1.00 1235 NZ LYS C 154 24.460 9.317 15.459 1.00 1236 C LYS C 154 24.460 9.317 15.459 1.00 1237 O LYS C 154 24.460 9.317 15.459 1.00 1238 N VAL C 155 22.410 10.749 15.692 1.00 1238 N VAL C 155 22.410 15.798 17.993 1.00 1239 CA VAL C 155 22.410 15.798 17.993 1.00 1230 CA LYS C 154 24.981 14.876 18.895 1.00 1231 CB VAL C 155 21.331 16.198 17.727 1.00 1232 CG LYS C 154 21.927 14.291 19.599 1.00 1233 CD LYS C 154 21.927 14.291 19.599 1.00 1234 CE LYS C 155 21.336 18.369 18.918 1.00 1236 C LYS C 155 21.336 18.369 18.918 1.00 1240 CB VAL C 155 21.336 18.369 18.918 1.00 1241 CG1 VAL C 155 21.336 18.369 18.918 1.00 1242 CG2 VAL C 155 21.336 18.369 18.918 1.00 1244 O VAL C 155 21.336 18.369 18.918 1.00 1245 CG TRP C 156 19.108 14.172 15.113 1.00 1246 CA TRP C 156 19.108 14.172 15.113 1.00 1247 CB TRP C 156 19.108 14.172 15.113 1.00 1248 CG TRP C 156 19.013 15.124 13.897 1.00 1249 CD2 TRP C 156 15.000 15.936 13.835 1.00 1251 CE3 TRP C 156 15.800 17.915 16.165 13.921 1.00 1252 CD1 TRP C 156 15.800 17.925 14.488 13.725 1.00 1253 NET TRP C 156 15.800 17.925 13.803 13.805 1.00 1254 CZ2 TRP C 156 15.600 15.936 13.835 1.00									1.00	149.34
1219								24.715	1.00	145.00
35 1220 CB THR C 152 30.034 17.838 22.951 1.00 1221 OG1 THR C 152 30.213 16.582 23.614 1.00 1222 CG2 THR C 152 31.182 18.762 23.334 1.00 1223 C THR C 152 27.631 17.343 23.278 1.00 1224 O THR C 152 27.631 17.343 23.278 1.00 1225 N GLY C 153 26.988 17.213 22.125 1.00 1226 CA GLY C 153 25.980 16.180 21.982 1.00 1227 C GLY C 153 25.515 15.979 20.558 1.00 1228 O GLY C 153 25.515 15.979 20.558 1.00 1229 N LYS C 154 24.759 14.905 20.345 1.00 1230 CA LYS C 154 24.759 14.905 20.345 1.00 1231 CB LYS C 154 24.531 13.110 18.710 1.00 1232 CG LYS C 154 24.531 13.110 18.710 1.00 1233 CD LYS C 154 24.531 13.110 18.710 1.00 1234 CE LYS C 154 24.531 13.110 18.710 1.00 1235 NZ LYS C 154 24.540 11.227 17.071 1.00 1236 C LYS C 154 24.540 11.227 17.071 1.00 1237 O LYS C 154 24.480 9.317 15.692 1.00 1238 N VAL C 155 22.748 14.876 18.895 1.00 1239 CA VAL C 155 22.748 14.876 18.895 1.00 1239 CA VAL C 155 22.410 15.798 17.993 1.00 1238 N VAL C 155 22.410 15.798 17.993 1.00 1239 CA VAL C 155 22.0918 17.729 17.614 1.00 1242 CG2 VAL C 155 21.031 16.198 17.727 1.00 1243 C VAL C 155 21.031 16.198 17.727 1.00 1244 CG1 VAL C 155 21.031 16.198 17.727 1.00 1249 CD2 TRP C 156 19.536 14.860 16.343 1.00 1249 CD2 TRP C 156 19.030 15.758 15.410 1.00 1249 CD2 TRP C 156 19.030 15.396 13.835 1.00 1249 CD2 TRP C 156 19.000 15.936 13.835 1.00 1251 CE3 TRP C 156 15.005 14.788 13.725 1.00 1252 CD1 TRP C 156 15.005 14.788 13.725 1.00 1253 NE1 TRP C 156 16.854 18.152 13.983 1.00							18.446		1.00	145.00
1222 CG2 THR C 152 31.182 18.762 23.334 1.00 1223 C THR C 152 27.631 17.343 23.278 1.00 1224 O THR C 152 27.631 17.343 23.278 1.00 1225 N GLY C 153 26.988 17.213 22.125 1.00 1226 CA GLY C 153 25.980 16.180 21.982 1.00 1227 C GLY C 153 25.515 15.979 20.558 1.00 1228 O GLY C 153 25.515 15.979 20.558 1.00 1229 N LYS C 154 24.759 14.905 20.345 1.00 1229 N LYS C 154 24.759 14.905 20.345 1.00 1231 CB LYS C 154 24.249 14.582 19.022 1.00 1232 CG LYS C 154 24.531 13.110 18.710 1.00 1232 CG LYS C 154 24.159 12.677 17.303 1.00 1233 CD LYS C 154 24.540 11.227 17.071 1.00 1234 CE LYS C 154 24.540 11.227 17.071 1.00 1235 NZ LYS C 154 24.460 9.317 15.692 1.00 1236 C LYS C 154 22.748 14.876 18.895 1.00 1237 O LYS C 154 22.748 14.876 18.895 1.00 1238 N VAL C 155 22.410 15.798 17.993 1.00 1238 N VAL C 155 21.031 16.198 17.727 1.00 1239 CA VAL C 155 21.031 16.198 17.727 1.00 1240 CB VAL C 155 21.031 16.198 17.727 1.00 1241 CG1 VAL C 155 21.031 18.198 17.727 1.00 1242 CG2 VAL C 155 21.031 18.198 17.727 1.00 1244 O VAL C 155 21.031 16.198 17.727 1.00 1245 N TRP C 156 19.500 18.129 17.274 1.00 1246 CA TRP C 156 19.536 14.880 16.343 1.00 60 1245 N TRP C 156 19.536 14.880 16.343 1.00 61 1246 CA TRP C 156 19.013 15.124 13.897 1.00 1249 CD2 TRP C 156 19.013 15.124 13.897 1.00 1251 CE3 TRP C 156 19.013 15.124 13.897 1.00 1252 CD1 TRP C 156 15.705 14.788 13.725 1.00 1253 NEI TRP C 156 15.705 14.788 13.725 1.00 1254 CC2 TRP C 156 15.6854 18.152 13.983 1.00	35		CB			30.034			1.00	154.69
1223 C THR C 152 27.631 17.343 23.278 1.00 1224 O THR C 152 27.420 16.609 24.240 1.00 1225 N GLY C 153 26.988 17.213 22.125 1.00 1226 CA GLY C 153 25.980 16.180 21.982 1.00 1227 C GLY C 153 25.980 16.180 21.982 1.00 1228 O GLY C 153 25.515 15.979 20.558 1.00 1229 N LYS C 154 24.759 14.905 20.345 1.00 1230 CA LYS C 154 24.249 14.582 19.022 1.00 1231 CB LYS C 154 24.531 13.110 18.710 1.00 1232 CG LYS C 154 24.531 13.110 18.710 1.00 1233 CD LYS C 154 24.540 11.227 17.071 1.00 1234 CE LYS C 154 24.540 11.227 17.071 1.00 1235 NZ LYS C 154 24.460 9.317 15.459 1.00 1236 C LYS C 154 24.460 9.317 15.459 1.00 1237 O LYS C 154 22.748 14.876 18.895 1.00 1238 N VAL C 155 22.410 15.798 17.993 1.00 1239 CA VAL C 155 22.410 15.798 17.993 1.00 1239 CA VAL C 155 22.410 15.798 17.993 1.00 1241 CG1 VAL C 155 21.031 16.198 17.727 1.00 1242 CG2 VAL C 155 21.031 16.198 17.727 1.00 1243 C C VAL C 155 20.918 17.729 17.614 1.00 1244 O VAL C 155 21.031 16.198 17.727 1.00 1245 C TAP C 156 19.536 14.860 16.343 1.00 1246 CA TRP C 156 19.536 14.860 16.343 1.00 1247 CB TRP C 156 19.003 14.172 15.113 1.00 1248 CG TRP C 156 19.003 14.172 15.113 1.00 1251 CE3 TRP C 156 18.0077 17.523 14.010 1.00 1252 CD1 TRP C 156 18.0077 17.523 14.010 1.00 1253 NE1 TRP C 156 18.0077 17.523 14.010 1.00 1254 CZ2 TRP C 156 18.0077 17.523 14.010 1.00 1254 CZ2 TRP C 156 18.0077 17.523 14.010 1.00 1254 CZ2 TRP C 156 18.0077 17.523 14.010 1.00 1254 CZ2 TRP C 156 18.0077 17.523 14.010 1.00			OG1	THR C		30.213			1.00	154.69
1224 O THR C 152 27.420 16.609 24.240 1.00 40 1225 N GLY C 153 26.988 17.213 22.125 1.00 1226 CA GLY C 153 25.980 16.180 21.982 1.00 1227 C GLY C 153 25.980 16.783 19.670 1.00 1228 O GLY C 153 25.830 16.783 19.670 1.00 1229 N LYS C 154 24.759 14.905 20.345 1.00 1220 CA LYS C 154 24.759 14.905 20.345 1.00 1231 CB LYS C 154 24.531 13.110 18.710 1.00 1232 CG LYS C 154 24.531 13.110 18.710 1.00 1233 CD LYS C 154 24.531 13.110 18.710 1.00 1234 CE LYS C 154 24.540 11.227 17.071 1.00 1235 NZ LYS C 154 24.460 10.749 15.692 1.00 1236 C LYS C 154 24.460 10.749 15.692 1.00 1237 O LYS C 154 24.460 19.317 15.459 1.00 1238 N VAL C 155 22.410 15.798 17.993 1.00 1238 N VAL C 155 22.410 15.798 17.993 1.00 1239 CA VAL C 155 20.918 17.729 17.614 1.00 1241 CG1 VAL C 155 20.918 17.729 17.614 1.00 1242 CG2 VAL C 155 21.336 18.369 18.918 1.00 1244 O VAL C 155 21.336 18.369 18.918 1.00 1245 N TRP C 156 19.508 14.860 16.343 1.00 1246 CA TRP C 156 19.508 14.860 16.343 1.00 1247 CB TRP C 156 19.018 14.172 15.113 1.00 1248 CG TRP C 156 19.018 14.172 15.113 1.00 1249 CD2 TRP C 156 19.018 14.172 15.113 1.00 1251 CE3 TRP C 156 18.0077 17.523 14.010 1.00 1253 NE1 TRP C 156 18.0077 17.523 14.010 1.00 1254 CZ2 TRP C 156 18.0077 17.523 14.010 1.00 1254 CZ2 TRP C 156 18.0077 17.523 14.010 1.00 1254 CZ2 TRP C 156 18.0077 17.523 14.010 1.00 1254 CZ2 TRP C 156 18.0077 17.523 14.010 1.00		1222	CG2							154.69
40 1225 N GLY C 153 26.988 17.213 22.125 1.00 1226 CA GLY C 153 25.980 16.180 21.982 1.0 1227 C GLY C 153 25.515 15.979 20.558 1.0 1228 O GLY C 153 25.515 15.979 20.558 1.0 1229 N LYS C 154 24.759 14.905 20.345 1.0 1230 CA LYS C 154 24.249 14.582 19.022 1.0 1231 CB LYS C 154 24.531 13.110 18.710 1.0 1232 CG LYS C 154 24.531 13.110 18.710 1.0 1233 CD LYS C 154 24.540 11.227 17.071 1.0 1234 CE LYS C 154 24.540 11.227 17.071 1.0 1235 NZ LYS C 154 24.480 9.317 15.459 1.0 1236 C LYS C 154 22.748 14.876 18.895 1.0 1237 O LYS C 154 22.748 14.876 18.895 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1238 N VAL C 155 22.410 15.798 17.727 1.0 1238 N VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 20.918 17.729 17.614 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.336 18.369 18.918 1.0 1245 C TRP C 156 19.536 14.860 16.343 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 61 1246 CA TRP C 156 19.536 14.860 16.343 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 16.550 15.936 13.835 1.0 1253 NE1 TRP C 156 16.550 15.936 13.835 1.0 1254 CZ2 TRP C 156 16.854 18.152 13.983 1.0										145.00 145.00
1226 CA GLY C 153 25.980 16.180 21.982 1.0 1227 C GLY C 153 25.515 15.979 20.558 1.0 1228 O GLY C 153 25.515 15.979 20.558 1.0 1229 N LYS C 154 24.759 14.905 20.345 1.0 45 1230 CA LYS C 154 24.249 14.582 19.022 1.0 1231 CB LYS C 154 24.531 13.110 18.710 1.0 1232 CG LYS C 154 24.531 13.110 18.710 1.0 1233 CD LYS C 154 24.540 11.227 17.071 1.0 1234 CE LYS C 154 24.540 11.227 17.071 1.0 1236 C LYS C 154 24.480 9.317 15.459 1.0 1237 O LYS C 154 22.480 9.317 15.459 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 21.031 16.198 17.727 1.0 1241 CG1 VAL C 155 20.918 17.729 17.614 1.0 1242 CG2 VAL C 155 21.031 16.198 17.727 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.336 18.369 18.918 1.0 1245 C C TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.536 14.860 16.343 1.0 1247 CB TRP C 156 19.536 14.860 16.343 1.0 1248 CG TRP C 156 19.108 14.172 15.113 1.0 1249 CD2 TRP C 156 19.108 14.172 15.113 1.0 1249 CD2 TRP C 156 19.108 14.172 15.113 1.0 1252 CD1 TRP C 156 15.869 17.203 13.878 1.0 1253 NEI TRP C 156 15.869 17.203 13.878 1.0 1253 NEI TRP C 156 15.869 17.203 13.878 1.0 1253 NEI TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 16.854 18.152 13.983 1.0	40									161.71
1227 C GLY C 153 25.515 15.979 20.558 1.0 1228 O GLY C 153 25.830 16.783 19.670 1.0 1229 N LYS C 154 24.759 14.905 20.345 1.0 45 1230 CA LYS C 154 24.249 14.582 19.022 1.0 1231 CB LYS C 154 24.531 13.110 18.710 1.0 1232 CG LYS C 154 24.59 12.677 17.303 1.0 1233 CD LYS C 154 24.540 11.227 17.071 1.0 1234 CE LYS C 154 24.540 10.749 15.692 1.0 1235 NZ LYS C 154 24.460 9.317 15.459 1.0 1236 C LYS C 154 22.748 14.876 18.895 1.0 1237 O LYS C 154 22.748 14.876 18.895 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 20.918 17.729 17.614 1.0 1242 CG2 VAL C 155 20.918 17.729 17.614 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.336 18.369 18.918 1.0 1245 C	40			GLY C						161.71
1228									1.00	161.71
1229 N LYS C 154 24.759 14.905 20.345 1.0 45 1230 CA LYS C 154 24.249 14.582 19.022 1.0 1231 CB LYS C 154 24.531 13.110 18.710 1.0 1232 CG LYS C 154 24.159 12.677 17.303 1.0 1233 CD LYS C 154 24.159 12.677 17.303 1.0 1234 CE LYS C 154 24.406 10.749 15.692 1.0 1235 NZ LYS C 154 24.406 9.317 15.459 1.0 1236 C LYS C 154 22.748 14.876 18.895 1.0 1237 O LYS C 154 22.748 14.876 18.895 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1238 N VAL C 155 21.031 16.198 17.727 1.0 55 1240 CB VAL C 155 21.031 16.198 17.727 1.0 1241 CG1 VAL C 155 20.918 17.729 17.614 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 1244 C T T T T T T T T T T T T T T T T T T			ŏ						1.00	161.71
45 1230 CA LYS C 154 24.249 14.582 19.022 1.0 1231 CB LYS C 154 24.531 13.110 18.710 1.0 1232 CG LYS C 154 24.159 12.677 17.303 1.0 1233 CD LYS C 154 24.540 11.227 17.071 1.0 1234 CE LYS C 154 24.540 11.227 17.071 1.0 1235 NZ LYS C 154 24.460 9.317 15.459 1.0 1236 C LYS C 154 22.748 14.876 18.895 1.0 1237 O LYS C 154 22.748 14.876 18.895 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 20.918 17.729 17.614 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.336 18.369 18.918 1.0 1245 N TRP C 156 19.536 14.860 16.343 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.108 14.172 15.113 1.0 1248 CG TRP C 156 19.108 14.172 15.113 1.0 1249 CD2 TRP C 156 19.00 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 18.077 17.523 14.010 1.0 1254 CZ2 TRP C 156 18.054 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0									1.00	155.18
1231 CB LYS C 154 24.531 13.110 18.710 1.0 1232 CG LYS C 154 24.159 12.677 17.303 1.0 1233 CD LYS C 154 24.540 11.227 17.071 1.0 1234 CE LYS C 154 24.106 10.749 15.692 1.0 1235 NZ LYS C 154 24.406 9.317 15.459 1.0 1236 C LYS C 154 22.748 14.876 18.895 1.0 1237 O LYS C 154 22.748 14.876 18.895 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 20.918 17.729 17.614 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.336 18.369 18.918 1.0 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.108 14.172 15.113 1.0 1248 CG TRP C 156 19.108 14.172 15.113 1.0 1249 CD2 TRP C 156 19.013 15.124 13.897 1.0 1249 CD2 TRP C 156 19.013 15.124 13.897 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 16.854 18.152 13.983 1.0 1253 NE1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 18.077 17.523 14.010 1.0 1254 CZ2 TRP C 156 18.077 17.523 14.010 1.0	45							19.022	1.00	155.18
1232	•••				154	24.531	13.110		1.00	249.69
1234 CE LYS C 154 24.106 10.749 15.692 1.0 50 1235 NZ LYS C 154 24.460 9.317 15.459 1.0 1236 C LYS C 154 22.748 14.876 18.895 1.0 1237 O LYS C 154 21.927 14.291 19.599 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 21.031 16.198 17.727 1.0 55 1240 CB VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 20.918 17.729 17.614 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.536 14.860 16.343 1.0 1247 CB TRP C 156 19.108 14.172 15.113 1.0 1248 CG TRP C 156 19.013 15.124 13.897 1.0 1249 CD2 TRP C 156 19.013 15.124 13.897 1.0 1249 CD2 TRP C 156 15.869 17.203 13.878 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 18.054 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0			CG		154	24.159			1.00	249.69
50 1235 NZ LYS C 154 24.460 9.317 15.459 1.0 1236 C LYS C 154 22.748 14.876 18.895 1.0 1237 O LYS C 154 21.927 14.291 19.599 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 22.410 15.798 17.993 1.0 55 1240 CB VAL C 155 21.031 16.198 17.727 1.0 55 1240 CB VAL C 155 21.031 16.198 17.727 1.0 1241 CG1 VAL C 155 20.918 17.729 17.614 1.0 1242 CG2 VAL C 155 19.500 18.129 17.274 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 <tr< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td>1.00</td><td>249.69</td></tr<>									1.00	249.69
1236 C LYS C 154 22.748 14.876 18.895 1.0 1237 O LYS C 154 21.927 14.291 19.599 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 21.031 16.198 17.727 1.0 55 1240 CB VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 19.500 18.129 17.274 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.108 14.172 15.113 1.0 1248 CG TRP C 156 19.013 15.124 13.897 1.0 1249 CD2 TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 18.054 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0										249.69
1237 O LYS C 154 21.927 14.291 19.599 1.0 1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 21.031 16.198 17.727 1.0 55 1240 CB VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 19.500 18.129 17.274 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 20.663 15.572 16.392 1.0 1244 O VAL C 155 20.663 15.572 16.392 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.108 14.172 15.113 1.0 1248 CG TRP C 156 19.013 15.124 13.897 1.0 1248 CG TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 16.500 15.936 13.835 1.0 65 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 15.705 14.788 13.725 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0	50									249.69
1238 N VAL C 155 22.410 15.798 17.993 1.0 1239 CA VAL C 155 21.031 16.198 17.727 1.0 1240 CB VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 19.500 18.129 17.274 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 20.663 15.572 16.392 1.0 1244 O VAL C 155 20.663 15.572 16.392 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.018 14.172 15.113 1.0 1248 CG TRP C 156 19.018 15.124 13.897 1.0 1249 CD2 TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 15.869 17.203 13.878 1.0 1253 NE1 TRP C 156 16.857 17.523 14.010 1.0 1253 NE1 TRP C 156 16.857 17.523 14.010 1.0 1253 NE1 TRP C 156 18.857 17.523 14.010 1.0										155.18 155.19
1239 CA VAL C 155 21.031 16.198 17.727 1.0 55 1240 CB VAL C 155 20.918 17.729 17.614 1.0 1241 CG1 VAL C 155 19.500 18.129 17.274 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 21.336 18.369 18.918 1.0 1244 O VAL C 155 20.663 15.572 16.392 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.018 14.172 15.113 1.0 1248 CG TRP C 156 19.018 15.124 13.897 1.0 1249 CD2 TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 18.5705 14.788 13.725 1.0 1253 NE1 TRP C 156 18.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 16.854 18.152 13.983 1.0		1237				21.827				207.77
55 1240 CB VAL C 155 20,918 17.729 17.614 1.0 1241 CG1 VAL C 155 19.500 18.129 17.274 1.0 1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 20.663 15.572 16.392 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.013 15.124 13.897 1.0 1248 CG TRP C 156 19.013 15.124 13.897 1.0 1249 CD2 TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 18.057 17.523 14.010 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0		1238		VAL C					1.00	207.77
1241	55								1.00	240.62
1242 CG2 VAL C 155 21.336 18.369 18.918 1.0 1243 C VAL C 155 20.663 15.572 16.392 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.013 15.124 13.897 1.0 1248 CG TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.869 17.203 13.878 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 18.054 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0	33								1.00	240.62
1243 C VAL C 155 20.663 15.572 16.392 1.0 1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.013 15.124 13.897 1.0 1248 CG TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.705 14.788 13.725 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0								18.918	1.00	240.62
1244 O VAL C 155 21.387 15.758 15.410 1.0 60 1245 N TRP C 156 19.536 14.860 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.013 15.124 13.897 1.0 1248 CG TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.705 14.788 13.725 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0							15.572	16.392	1.00	207.77
60 1245 N TRP C 156 19.536 14.880 16.343 1.0 1246 CA TRP C 156 19.108 14.172 15.113 1.0 1247 CB TRP C 156 19.013 15.124 13.897 1.0 1248 CG TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.705 14.788 13.725 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0					155		15.758		1.00	207.77
1247 CB TRP C 156 19.013 15.124 13.897 1.0 1248 CG TRP C 156 17.915 16.165 13.921 1.0 1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.705 14.788 13.725 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0	60	1245		TRP C					1.00	218.56
1248		1246		TRP C					1.00	218.56
1249 CD2 TRP C 156 16.500 15.936 13.835 1.0 65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.705 14.788 13.725 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0				TRP C					1.00	249.69 249.69
65 1250 CE2 TRP C 156 15.869 17.203 13.878 1.0 1251 CE3 TRP C 156 15.705 14.788 13.725 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0				TRP C					1.00 1.00	249.69
1251 CE3 TRP C 156 15.705 14.788 13.725 1.0 1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0	65								1.00	249.69
1252 CD1 TRP C 156 18.077 17.523 14.010 1.0 1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0	UJ			TRP					1.00	249.69
1253 NE1 TRP C 156 16.854 18.152 13.983 1.0 1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0									1.00	249.69
1254 CZ2 TRP C 156 14.481 17.354 13.816 1.0		1253		TRP C					1.00	249.69
		1254		TRP C					1.00	249.69
1.1 1000.01 GEGS 14.003 17.00 1.1.	70	1255	CZ3	TRP C	156	14.324	14.939	13.660	1.00	249.69

	1256	CH2	TRP C	156	13.728	16.214	13.709	1.00	249.69
	1257	Č.	TRP C	156	20.213	13.163	14.835	1.00	218.56
	1258	Ŏ	TRP C	156	20.243	12.080	15.416	1.00	218.56
	1259	N	GLN C	157	21.130	13.548	13.949	1.00	165.87
5	1260	CA	GLN C	157	22.264	12.707	13.578	1.00	165.87
-	1261	СВ	GLN C	157	21.918	11.902	12.321	1.00	216.87
	1262	CG	GLN C	157	20.967	10.737	12.583 13.496	1.00	216.87
	1263	CD	GLN C	157	21.564	9.669	13.450	1.00 1.00	216.87 216.87
	1264	OE1	GLN C	157	22.561	9.032 9.468	14.661	1.00	216.87
10	1265	NE2	GLN C	157	20.951		13.378	1.00	165.87
	1266	Ç	GLN C	157	23.592	13.461 12.979	12.705	1.00	165.87
	1267	0	GLN C	157	24.495	14.648	13.960	1.00	219.11
	1268	N.	LEU C	158	23.706 24.940	15.419	13.858	1.00	219.11
	1269	CA	LEU C	158	24.767	16.628	12.929	1.00	248.45
15	1270	CB	LEU C	158 158	24.766	16.392	11.415	1.00	248.45
	1271	CG	LEU C	158	25.460	17.580	10.748	1.00	248.45
	1272	CD1	LEU C	158	25.498	15.110	11.054	1.00	248.45
	1273	CD2	LEU C	158	25.415	15.892	15.230	1.00	219.11
20	1274	C O	LEU C	158	24.619	16.116	16.136	1.00	219.11
20	1275	N	ASP C	159	26.724	16.040	15.374	1.00	202.98
	1276 1277	CA:	ASP C	159	27.314	16.485	16.629	1.00	202.98
	1277	CB	ASP C	159	28.746	15.957	16.757	1.00	249.69
		CG	ASP C	159	28.834	14.458	16.563	1.00	249.69
25	1279 1280	OD1	ASP C	159	28.215	13.718	17.356	1.00	249.69
23	1281	OD2	ASP C	159	29.522	14.017	15.616	1.00	249.69
	1282	C	ASP C	159	27.341	18.007	16.704	1.00	202.98
	1283	ŏ	ASP C	159	27.474	18.690	15.682	1.00	202.98
	1284	Ň	TYR C	160	27.209	18.541	17.915	1.00	193.11
30	1285	CA	TYR C	160	27.246	19.988	18.104	1.00	193.11
50	1286	CB	TYR C	160	25.852	20.584	18.043	1.00	187.38
	1287	ČĢ	TYR C	160	25.114	20.253	16.778	1.00	187.38
	1288	CD1	TYR C	160	24.305	19.113	16.702	1.00	187.38
	1289	CE1	TYR C	160	23.579	18.813	15.553	1.00	187.38
35	1290	CD2	TYR C	160	25.195	21.087	15.665	1.00	187.38
75	1291	CE2	TYR C	160	24.479	20.796	14.504	1.00	187.38
	1292	CZ	TYR C	160	23.666	19.657	14.458	1.00	187.38
	1293	OH	TYR C	160	22.920	19.374	13.337	1.00	187.38
	1294	С	TYR C	160	27.895	20.388	19.413	1.00	193.11
40	1295	0	TYR C	160	27.769	19.705	20.429	1.00	193.11 171.02
	1296	N	GLU C	161	28.585	21.519	19.360	1.00 1.00	171.02
	1297	CA	GLU C	161	29.296	22.064	20.494	1.00	238.76
	1298	CB	GLU C	161	30.740	22.358	20.052 21.085	1.00	238.76
	1299	CG	GLU C	161	31.660	22.975	20.671	1.00	238.76
45	1300	CD	GLU C	161	33.121	22.878	21.196	1.00	238.76
	1301	OE1	GLU C	161	33.948	23.655 22.015	19.827	1.00	238.76
	1302	OE2	GLU C	161	33.445	23.321	20.952	1.00	171.02
	1303	Ç	GLU C	161	28.560	24.068	20.135	1.00	171.02
~^	1304	0	GLU C	161	28.044	23.533	22.263	1.00	160.21
50	1305	N	SER C	162	28.500 27.820	24.693	22.840	1.00	160.21
	1306	CA	SER C	162	27.182	24.308	24.174	1.00	143.02
	1307	CB	SER C	162	28.169	23.903	25.109	1.00	143.02
	1308	OG	SER C	162	28.767	25.856	23.078	1.00	160.21
<i></i>	1309	C	SER C	162 162	29.978	25.678	23.147	1.00	160.21
55	1310	0	SER C	163	28.211	27.053	23.200	1.00	142.78
	1311	N	GLU C	163	29.043	28.207	23.471	1.00	142.78
	1312	CA	GLU C	163	28.195	29.492	23.498	1.00	247.65
•	1313	CB CG	GLU C	163	27.742	30.009	22.130	1.00	247.65
60	1314		GLU C	163	28.870	30.651	21.331	1.00	247.65
60	1315	CD OF1	GLU C	163	29.506	31.604	21.841	1.00	247.65
	1316	OE1 OE2	GLU C	163		30.207	20.189	1.00	247.65
	1317		GLU C	163		27.931	24.857	1.00	142.78
	1318	C	GLU C	163		27.254	25.666	1.00	142.78
65	1319	N	PRO C	164		28.429	25.144	1.00	104.76
03	1320	CD	PRO C	164		29,158	24.241	1.00	198.66
	1321	CA	PRO C	164		28.209	26.442	1.00	104.76
	1322 1323	CB	PRO C	164		28.445	26.144	1.00	198.66
	1323	CG	PRO C	164		29.581	25.180	1.00	198.66
70	1325	č	PRO C	164		29.170	27.501	1.00	104.76
70	انعدا	•			_				

						00.019	27.189	1.00	104.76
	1326	0		164	30.623	30.318 28.719	28.751	1.00	150.81
	1327	N		165	30.872	29.562	29.820	1.00	150.81
	1328	CA;	LEU C	165	30.352 28.962	29.067	30.202	1.00	114.56
	1329	СВ	LEU C	165	28.295	29.843	31.329	1.00	114.56
5	1330	CG	LEU C	165 165	28.627	31.336	31.179	1.00	114.56
	1331	CD1	LEU C	165	26.778	29.5ªE	31.296	1.00	114.56
	1332	CD2	LEU C	165	31.213	29.644	31.065	1.00	150.81 150.81
	1333	C	LEU C	165	31.648	28.620	31.589 31.538	1.00 1.00	123.03
10	1334	N	ASN C	166	31.445	30.864	31.550	1.00	123.03
10	1335 1336	CA	ASN C	166	32.247	31.058	32.716	1.00	146.40
	1337	СВ	ASN C	166	32.969	32.409 32.314	32.177	1.00	146.40
	1338	CG	ASN C	166	34.388	31.273	32.254	1.00	146.40
	1339	OD1	ASN C	166	35.031 34.888	33.429	31.660	1.00	146.40
15	1340	ND2	ASN C	166 166	31.402	30.985	34.019	1.00	123.03
	1341	C	ASN C ASN C	166	30.257	31.409	34.022	1.00	123.03
	1342	0	ILE C	167	31.976	30.458	35.103	1.00	149.03 149.03
	1343	N CA	ILE C	167	31.266	30.3 2 0	36.374	1.00	98.22
20	1344	CB	ILE C	167	30.670	28.946	36.551	1.00 1.00	98.22
20	1345 1346	CG2	ILE C	167	30.085	28.799	37.947 35.473	1.00	98.22
	1347	CG1	ILE C	167	29.610	28.707 27.336	35.526	1.00	98.22
	1348	CD1	ILE C	-167	29.025	30.592	37.548	1.00	149.03
	1349	С	ILE C	167	32.178	29.983	37.667	1.00	149.03
25	1350	0	ILE C	167	33.233 31.755	31.471	38.440	1.00	107.43
	1351	N	THR C	168 168	32,586	31.792	39.591	1.00	107.43
	1352	CA	THR C	168	33,120	33.225	39.487	1.00	120.91 120.91
	1353	CB OG1	THR C	168	33.823	33.372	38.246	1.00	120.91
20	1354	CG2	THR C	168	34.054	33.526	40.633	1.00 1.00	107.43
30	1355 1356	C	THR C	168	31.955	31.603	40.965 41.312	1.00	107.43
	1357	ŏ	THR C	168	30.943	32.192 30.761	41.750	1.00	107.46
	1358	N	VAL C	169	32.594	30.470	43.092	1.00	107.46
	1359	CA	VAL C	169	32,152 32,206	28.935	43,374	1.00	105.06
35	1360	СВ	VAL C	169 169	32.281	28.657	44.853	1.00	105.06
	1361	CG1	VAL C VAL C	169		28.269	42.794	1.00	105.06
	1362	CG2	VAL C VAL C	169		31.217	44.025	1.00	107.46 107.46
	1363	C	VAL C	169		30.874	44.135	1.00 1.00	143.55
40	1364 1365	N	ILE C	170	32.548	32.248	44.677 45.614	1.00	143.55
40	1366	ČA	ILE C	170		33.068 34.549	45.488	1.00	150.86
	1367	СВ	ILE C	170		34.967	44.028	1.00	150.86
	1368	CG2	ILE C	170		34.741	46.000	1.00	150.86
	1369	CG1	ILE C	170 170		36.188	45.961	1.00	150.86
45	1370	CD1	ILE C	17		32.586	47.056	1.00	143.55 143.55
	1371	C	ILE C	17		31.824	47.309	1.00	170.19
	1372	0 N	LYS C	17		33.028	47.994	1.00 1.00	170.19
	1373	CA	LYS C	17	1 33.795	32.588	49.379 49.790	1.00	247.79
50	1374) 1375	CB	LYS C	17		31.812	49.598	1.00	247.79
50	1376	CG	LYS C	17		32.611 31.712	49.375	1.00	247.79
	1377	CD	LYS C	17		30.756	50.537	1.00	247.79
	1378	CE	LYS C	17		29.921	50.335	1.00	247.79
	1379	NZ	LYS C	17 17		33.715	50.378		170.19 170.19
5:		C	LYS C		71 33.540	33.498	51.596		249.69
	1381	0 C1	NAG C		21 5.113	30.265	25.361		249.69
	1382 1383	C2	NAG C		21 5.275	28.765	25.132 24.798		249.69
	1384	N2	NAG C		21 6.660	28.481	25.015		249.69
6	0 1385	C7	NAG C		21 7.164	27. 267 26.331	25.485		249.69
U	1386	07	NAG C	_	21 6.500 21 8.624	27.050	24.648		249.69
	1387	C8	NAG C			28.288	24.010	1.00	249.69
	1388	cs	NAG C	_	21 4.349 21 4.386	26.868	23.92		249.69
	1389	03	NAG C		21 2.899	28.741	24.221		249.69 249.69
6	5 1390	C4	NAG C	_	21 2.183	28.474	23.00		249.69 249.69
	1391	O4 C5	NAG C		221 2.851	30.255	24.55		249.69
	1392	O5	NAG C		221 3.741	30.568	25.65 24.97		249.69
	1393 1394	C6	NAG (•	221 1.472		26.08		249.69
•	70 1395	06	A NAG	2	221 0.977	30.009	25.50		
,									

1

	1396 1397	C1 C2	NAG C	222 222	0.788 0.312	28.434 27.230	23.006 22.166	1.00 1.00	249.69 249.69
	1398	N2 .	NAG C	222	0.806	25.988	22.749	1.00	249.69
5	1399 1400	C7 O7	NAG C	222	-0.041	25.044	23.166	1.00	249.69
,	1401	C8	NAG C NAG C	222 222	-1.270 0.570	25.153 23.783	23.088	1.00	249.69
	1402	င်ဒိ	NAG C	222	0.819	23.763 27.382	23.761 20.711	1.00 1.00	249.69
	1403	03	NAG C	222	0.285	26.347	19.894	1.00	249.69
10	1404	C4	NAG C	222	0.422	28.755	20.130	1.00	249.69 249.69
10	1405	04	NAG C	222	1.038	28.935	18.860	1.00	249.69
	1406 1407	C5 O5	NAG C	222	0.860	29.881	21.083	1.00	249.69
	1408	C6	NAG C NAG C	222 222	0.308 0.423	29.658	22.408	1.00	249.69
	1409	06	NAG C	222	1.512	31.266 32.185	20.635 20.656	1.00	249.69
15	1410	C1	NAG C	242	18.968	46.404	25.932	1.00 1.00	249.69 249.69
	1411	C2	NAG C	242	18.118	46.230	24.662	1.00	249.69
	1412	N2	NAG C	242	16.700	46.211	24.968	1.00	249.69
	1413 1414	C7 O7	NAG C	242	15.905	47.139	24.446	1.00	249.69
20	1415	∃8	NAG C NAG C	242 242	16.318 14.433	48.033 47.071	23.707	1.00	249.69
	1416	C3	NAG C	242	18.532	44.931	24.794 23.964	1.00 1.00	249.69
	1417	O3	NAG C	242	17.775	44.760	22.773	1.00	249.69 249.69
	1418	C4	NAG C	242	20.036	44.983	23.636	1.00	249.69
25	1419	04	NAG C	242	20.457	43.699	23.125	1.00	249.69
25	1420 1421	C5 O5	NAG C	242	20.872	45.340	24.894	1.00	249.69
	1422	C6	NAG C NAG C	242 242	20.352 22.318	46.526 45.643	25.559	1.00	249.69
	1423	06	NAG C	242	23.194	45.643 44.624	24.539 24.998	1.00 1.00	249.69
••	1424	C1	NAG C	243	21.000	43.678	21.849	1.00	249.69 249.69
30	1425	C2	NAG C	243	21.827	42.403	21.660	1.00	249.69
	1426 1427	N2	NAG C	243	22.908	42.331	22.621	1.00	249.69
	1428	C7 O7	NAG C NAG C	243	23.110	41.201	23.298	1.00	249.69
	1429	C8	NAG C	243 243	22.404 24.264	40.193 41.186	23.157 24.287	1.00	249.69
35	1430	C3	NAG C	243	22.382	42.377	20.246	1.00 1.00	249.69
	1431	03	NAG C	243	23.150	41.195	20.045	1.00	249.69 249.69
	1432	C4	NAG C	243	21.223	42.406	19.276	1.00	249.69
	1433 1434	O4 C5	NAG C	243	21.794	42.333	17.983	1.00	249.69
40	1435	O5	NAG C NAG C	243 243	20.366 19.915	43.682	19.518	1.00	249.69
	1436	C6	NAG C	243	19.112	43.690 43.738	20.906 18.662	1.00 1.00	249.69
	1437	O6	NAG C	243	18.229	42.666	18.966	1.00	249.69 249.69
	1438	C1	MAN C	244	21.150	41.717	16.941	1.00	247.75
45	1439 1440	C2 O2	MAN C	244	21.485	42.608	15.841	1.00	247.75
43	1441	C3	MAN C MAN C	244 244	22.880 21.041	42.966	15.943	1.00	247.75
	1442	O3	MAN C	244	21.229	42.012 42.927	14.541 13.482	1.00 1.00	247.75
	1443	C4	MAN C	244	21.699	40.671	14.305	1.00	247.75 247.75
50	1444	04	MAN C	244	21.301	40.157	13.050	1.00	247.75
50	1445	C5	MAN C	244	21.269	39.743	15.442	1.00	247.75
	1446 1447	O5 C6	MAN C MAN C	244	21.734	40.330	16.721	1.00	247.75
	1448	06	MAN C	244 244	21.705 23.038	38.271 38.030	15.255 15.676	1.00	247.75
	1449	C1	NAG C	250	0.024	39.200	37.140	1.00 1.00	247.75
55	1450	C2	NAG C	250	-0.633	37.995	37.P 14	1.00	249.69 249.69
	1451	N2	NAG C	250	-0.363	38.033	39.271	1.00	249.69
	1452 1453	C7	NAG C	250	-1.342	38.313	40.126	1.00	249.69
	1454	O7 C8	NAG C NAG C	250 250	-2.500 -0.985	38.550	39.764	1.00	249.69
60	1455	ČŠ	NAG C	250	-0.965 -0.084	38.336 36.691	41.607 37.242	1.00	249.69
	1456	O 3	NAG C	250	-0.751	35.573	37.814	1.00 1.00	249.69 249.69
	1457	Ç4	NAG C	250	-0.273	36.691	35.716	1.00	249.69
	1458	04 05	NAG C	250	0.355	35.542	35.160	1.00	249.69
65	1459 1460	C5 O5	NAG C	250	0.338	37.973	35.105	1.00	249.69
J J	1461	C6	NAG C NAG C	250 250	-0.235 0.100	39.149	35.731	1.00	249.69
	1462	06	NAG C	250 250	0.100	38.106 39.435	33.606 33.163	1.00	249.69
	1463	C1	NAG C	274	17.463	53.378	50.102	1.00 1.00	249.69
70	1464	C2	NAG C	274	18.624	52.801	50.945	1.00	249.69 249.69
70	1465	N2	NAG C	274	18.123	51.805	51.883	1.00	249.69

			NAC C	27,4	18.919	50.834	52.330	1.00	249.69
	1466	C7	NAG C NAG C		20.099	50.723	51.992	1.00	249.69
	1467	07	NAG C	274	18.316	49.836	53.303	1.00	249.69
	1468	C8 C3	NAG C	274	19.337	53.945	51.704	1.00	249.69
~	1469	03	NAG C	274	20.487	53.442	52.377	1.00	249.69
	1470 1471	C4	NAG C	274	19.755	55.062	50.730	1.00	249.69 249.69
	1472	04	NAG C	274	20.286	56.164	51.457 49.899	1.00 1.00	249.69
	1473	C5	NAG C	274	18.548	55.520	49.203	1.00	249.69
	1474	O5	NAG C	274	17.957	54.391	48.849	1.00	249.69
10	1475	C6	NAG C	274	18.929	56.550 56.817	47.970	1.00	249.69
	1476	O 6	NAG C	274	17.844 16.958	19.435	32.669	1.00	249.69
	1477	C1	NAG C	335 335	15.937	19.674	33.820	1.00	249.69
	1478	C2	NAG C NAG C	335	16.535	19.244	35.073	1.00	249.69
16	1479	N2 C7	NAG C	335	16.783	20.124	36.042	1.00	249.69
15	1480 1481	07	NAG C	335	16.517	21.327	35.947	1.00	249.69 249.69
	1482	C8	NAG C	335	17.416	19.588	37.314	1.00 1.00	249.69
	1483	C3	NAG C	335	14.586	18.951	33.638 34.457	1.00	249.69
	1484	03	NAG C	335	13.605	19.572	32.190	1.00	249.69
20	1485	C4	NAG C	335	14.117	18.995 18.250	32.042	1.00	249.69
	1486	04	NAG C	335	12.912 15.219	18.405	31.318	1.00	249.69
	1487	C5	NAG C NAG C	335 335	16.370	19.273	31.353	1.00	249.69
	1488	O5	NAG C	335	14,799	18.275	29.862	1.00	249.69
25	1489	C6 O6	NAG C	335	14.956	16.942	29.398	1.00	249.69
25	1490 1491	C1	NAG C	340	29.647	21.246	52.250	1.00	249.46 249.46
	1492	C2	NAG C	340	30.433	22.313	53.032	1.00 1.00	249.46
	1493	N2	NAG C	340	30.974	23.304	52.117 52.373	1.00	249.46
	1494	C7	NAG C	340	30.836	24.605 25.044	53.381	1.00	249.46
30	1495	07	NAG C	340	30.269	25.569	51.356	1.00	249.46
	1496	C8	NAG C	340	31.425 31.568	21.625	53.818	1.00	249.46
	1497	C3	NAG C NAG C	340 340	32.255	22.575	54.628	1.00	249.46
	1498	03	NAG C	340	30.996	20.503	54.702	1.00	249.46
25	1499	C4 O4	NAG C	340	32.063	19.789	55.308	1.00	249.46
35	1500 1501	C5	NAG C	340	30.136	19.545	53.853	1.00	249.46 249.46
	1502	O5	NAG C	340	29.101	20.280	53.154 54.660	1.00 1.00	249.46
	1503	C6	NAG C	340	29.442	18.463	53.851	1.00	249.46
	1504	O 6	NAG C	340	28.518	17.737 33.414	30.999	1.00	209.37
40	1505	C 1	NAG C	366	36.171 38.136	34.345	29.797	1.00	209.37
	1506	C2	NAG C NAG C	366 366	35.092	33.912	28.886	1.00	209.37
	1507	N2	NAG C	366	33.862	34.405	28.999	1.00	209.37
	1508	C7 O7	NAG C	366	33.555	35.244	29.848	1.00	209.37 209.37
45	1509 1510	C8	NAG C	366	32.813	33.903	28.017	1.00 1.00	209.37
43	1511	Čŝ	NAG C	366		34.322	29.088 28.073	1.00	209.37
	1512	O3	NAG C	366		35.319 34.557	30.067	1.00	209.37
	1513	C4	NAG C	366		34.256	29.386	1.00	209.37
	1514	Q4	NAG C	366 366		33.652	31.302	1.00	209.37
50	1515	C5	NAG C NAG C	366		33.813	31.891	1.00	209.37
	1516	O5 C6	NAG C	366		33.935	32.390	1.00	209.37
	1517	C6 O6	NAG C	366		32.957	33.413	1.00	209.37
	1518 1519	C1	NAG C	367		35.232	29.397	1.00	249.69 249.69
55	1520	C2	NAG C	367		34.596	29.111 30.070	1.00 1.00	249.69
55	1521	N2	NAG C	36		33.546 32.277	29.668	1.00	249.69
	1522	C7	NAG C	36		31.931	28.498	1.00	249.69
	1523	07	NAG C	36		31.227	30.725	1.00	249.69
	1524	C8	NAG C NAG C	36 36		35.695	29.166	1.00	249.69
60	1525	C3	NAG C			35.149	28.892	1.00	249.69
	1526	03 C4	NAG C			36.779	28.132	1.00	249.69 249.69
	1527 1528	64	NAG C		7 43.876	37.854	28.245	1.00	249.69
	1529	C5	NAG C	36		37.296	28.348	1.00 1.00	249.69
65	1530	O5	NAG C	36		36.196	28.373 27.251	1.00	249.69
	1531	C6	NAG C			38.236 37.661	26.474		249.69
	1532	O6	NAG C			19.933	14.932		249.69
	1533	CB	LYS A			21.022	14.456		249.69
~	1534	CG	LYS A		2.217		15.610		249.69
70) 1535	CD	בוס ר	•					

	1536	CE	LYS A	4.	1.292	22.987	15.108	1.00	249.69
	1537	NZ	LYS A	4	0.762 5.030	23.841 20.019	16.212 12.832	1.00 1.00	249.69 249.22
	1538	C:	LYS A LYS A	4	5.450	21.116	13.205	1.00	249.22 249.22
5	1539 1540	Ň	LYS A	4	5.205	18.061	14.356	1.00	249.22
,	1541	ĊA	LYS A	4	4.291	19.100	13.797	1.00	249.22
	1542	N	PRO A	5	5.213	19.581	11.582	1.00	249.41
	1543	CD	PRO A	5	4.979	18.215	11.068	1.00	133.18
	1544	CA	PRO A	5	5.912	20.398	10.589	1.00	249.41
10	1545	СВ	PRO A	5	6.459 5.376	19.360 18.335	9.606 9.599	1.00 1.00	133.18 133.18
	1546	C CG	PRO A PRO A	5 5	5.376 4.969	21.407	9.927	1.00	249.41
	1547 1548	ŏ	PRO A	5	3.754	21.219	9.927	1.00	249.41
	1549	Ň	LYS A	6	5.529	22.477	9.377	1.00	196.60
15	1550	CA	LYS A	6	4.724	23.489	8.709	1.00	196.60
	1551	CB	LYS A	6	4.429	24.652	9.660	1.00	249.69
	1552	CG	LYS A	6	3.524	25.719	9.050 10.067	1.00 1.00	249.69
	1553	CD	LYS A LYS A	6 6	3.113 2.180	26.783 27.812	9.436	1.00	249.69 249.69
20	1554 1555	CE NZ	LYS A LYS A	6	1.664	28.800	10.424	1.00	249.69
20	1556	Ċ	LYS A	6	5.433	24.000	7.458	1.00	196.60
	1557	ŏ	LYS A	6	6.478	24.664	7.539	1.00	196.60
	1558	N	VAL A	7	4.850	23.695	6.304	1.00	192.34
~ ~	1559	CA	VAL A	7	5.416	24.094	5.029	1.00	192.34
25	1560	CB	VAL A	7	4.656 5.470	23.429 23.549	3.870 2.587	1.00 1.00	160.27 160.27
	1561	CG1 CG2	VAL A VAL A	7 7	4. 363	21.983	4.195	1.00	160.27
	1562 1563	C	VAL A	7	5.403	25.607	4.807	1.00	192.34
	1564	ŏ	VAL. A	7	4.350	26.253	4.868	1.00	192.34
30	1565	N	SER A	8	6.582	26.165	4.544	1.00	184.23
	1566	CA	SER A	8	6.726	27.594	4.284	1.00	184.23
	1567	CB	SER A	8	7.897	28.148	5.099	1.00 1.00	230.08 230.08
	1568	OG C	SER A SER A	8 8	9.063 6.978	27.354 27.814	4.945 2.789	1.00	184.23
35	1569 1570	ŏ	SER A	8	7.389	26.889	2.087	1.00	184.23
33	1571	Ň	LEU A	9	6.726	29.025	2.297	1.00	167.11
	1572	CA	, LEU A	9	6.948	29.312	0.880	1.00	167.11
	1573	CB	LEU A	9	5.626	29.535	0.147	1.00	178.21
40	1574	CG	LEU A	9	4.541	28.451	0.105	1.00 1.00	178.21 178.21
40	1575	CD1	LEU A LEU A	9 9	3.549 5.128	28.821 27.083	-0.980 -0.188	1.00	178.21
	1576 1577	CD2 C	LEU A	9	7.817	30.533	0.666	1.00	167.11
	1578	ŏ	LEU A	9	7.946	31.373	1.552	1.00	167.11
	1579	N	ASN A	10	8.405	30.629	-0.522	1.00	147.32
45	1580	CA	ASN A	10	9.260	31.769	-0.855	1.00	147.32
	1581	CB	ASN A	10	10.634	31.610	-0.219	1.00	249.69
	1582	ÇG OD1	ASN A ASN A	10 10	11.421 11.028	32.902 33.886	-0.234 0.395	1.00 1.00	249.69 249.69
	1583 1584	OD1 ND2	ASN A	10	12.534	32.911	-0.959	1.00	249.69
50	1585	C	ASN A	10	9.396	31.902	-2.374	1.00	147.32
50	1586	ŏ	ASN A	10	10.037	31.073	-3.022	1.00	147.32
	1587	N	PRO A	11	8.851	32.979	-2.953	1.00	237.62
	1588	CD	PRO A	11	8.944	33.177	-4.413 0.043	1.00	161.80
55	1589	CA	PRO A	11	8.057 7.554	34.058 34.834	-2.348 -3.552	1.00 1.00	237.62 161.80
55	1590 1591	CB CG	PRO A PRO A	11 11	8.646	34.638	-4.548	1.00	161.80
	1592	č	PRO A	11	6.921	33.599	-1.438	1.00	237.62
	1593	ŏ	PRO A	11	6.554	32.428	-1.435	1.00	237.62
	1594	N	PRO A	12	6.338	34.529	-0.662	1.00	147.54
60	1595	CD	PRO A	12	6.781	35.905	-0.441	1.00	140.19
	1596	CA	PRO A	12	5.229	34.189	0.236	1.00 1.00	147.54 140.19
	1597	CB CG	PRO A PRO A	12 12	5.107 6.465	35.433 36.081	1.112 1.016	1.00	140.19
	1598 1599	Č	PRO A	12	3.967	33.943	-0.572	1.00	147.54
65	1600	ŏ	PRO A	12	3.063	33.202	-0.148	1.00	147.54
	1601	Ň	TRP A	13	3.929	34.576	-1.744	1.00	165.94
	1602	CA	TRP A	13	2.824	34.492	-2.698	1.00	165.94
	1603	CB	TRP A	13	3.247	35.209	-3.968	1.00	139.27
70	1604	CG	TRP A	13 13	3.825	36.552 37.438	-3.699 -2.648	1.00 1.00	139.27 139.27
70	1605	CD2	TRP A	13	3.455	37.730	-2.040	1.00	107.2/

	1606	CE2		13	4.233 2.546	38.603 37.363		1.00 1.00	139.27 139.27
	1607	CE3	TRP A	13	4.784	37.201	-4.428	1.00	139.27
	1608	CD1	TRP A	13	5.035	38.438	-3.891	1.00	139.27
	1609	NE1.	TRP A	13 13	4.122	39.682	-1.917	1.00	139.27
5	1610	CZ2	TRP A	13	2.433	38.434	-0.731	1.00	139.27 139.27
	1611	CZ3 CH2	TRP A	13	3.218	39.577	-0.892	1.00 1.00	165.94
	1612	C	TRP A	13	2.428	33.061	-3.048 -3.663	1.00	165.94
	1613 1614	ŏ	TRP A	13	3.219	32.342 32.652	-2.689	1.00	109.00
10	1615	N	ASN A	14	1.213 0.782	31.293	-2.990	1.00	109.00
10	1616	CA	ASN A	14	0.762	30.660	-1.746	1.00	167.27
	1617	CB	ASN A ASN A	14 14	-1.091	31.352	-1.312	1.00	167.27 167.27
	1618	CG OD1	ASN A	14	-1.088	32.556	-1.050	1,00 1,00	167.27
15	1619 1620	ND2	ASN A	14	-2.188	30.596	-1.234 -4.164	1.00	109.00
13	1621	C	ASN A	14	-0.200	31.224 30.275	-4.295	1.00	109.00
	1622	0	ASN A	14	-0.981 -0.153	32.255	-5.006	1.00	160.32
	1623	N	ARG A	15 15	-0.977	32.384	-6.220	1.00	160.32
	1624	CA	ARG A ARG A	15	-2.094	33.426	-6.042	1.00	119.95 119.95
20	1625	CB CG	ARG A	15	-2.974	33.286	-4.790 -4.834	1.00 1.00	119.95
	1626 1627	CD	ARG A	15	-4.127	34.296	-4.834 -5.737	1.00	119.95
	1628	NE	ARG A	15	-5.205	33.881 34.709	-6.500	1.00	119.95
	1629	CZ	ARG A	15	-5.920 -5.674	36.015	-6.492	1.00	119.95
25	1630	NH1	ARG A	15 15	-5.874 -6.894	34.239	-7.267	1.00	119.95
	1631	NH2	ARG A ARG A	15	0.012	32.914	-7.260	1.00	160.32 160.32
	1632	C O	ARG A	15	0.338	34.098	-7.259	1.00 1.00	135.68
	1633	N	ILE A	16	0.490	32.054	-8.148 -9.124	1.00	135.68
30	1634 1635	ĊA	ILE A	16	1.479	32.491 31.783	-8.904	1.00	134.22
50	1636	СВ	ILE A	16	2.803 3.532	32.401	-7.704	1.00	134.22
	1637	CG2	ILE A	16 16	2.534	30.272	-8.762	1.00	134.22
	1638	CG1	ILE A ILE A	16	3.763	29.404	-8.762	1.00	134.22 135.68
25	1639	CD1 C	ILE A	16	1.141	32.283	-10.581 -10.938	1.00 1.00	135.68
35	1640 1641	ŏ	ILE A	16	0.358	31.408	-11.425	1.00	145.71
	1642	Ň	PHE A	17	1.774	33.090 33.015	-12.870	1.00	145.71
	1643	CA	PHE A	17	1.589 2.211	34.246	-13.547	1.00	146.10
	1644	CB	PHE A PHE A	17 17	1.276	35.401	-13.687	1.00	146.10 146.10
40	1645	CG	PHE A	17	1.752	36.702	-13.601	1.00 1.00	146.10
	1646	CD1 CD2	PHE A	17	-0.067	35.195	-13.957 -13.781	1.00	146.10
	1647 1648	CE1	PHE A	17	0.901	37.798 36.273	-14.142	1.00	146.10
	1649	CE2	PHE A	17	-0.927	37.586	-14.054	1.00	146.10
45	1650	CZ	PHE A	17 17	-0.437 2.240	31.744	-13.417	1.00	145.71
	1651	Ç	PHE A PHE A	17	2.882	30.991	-12.692	1.00	145.71 190.00
	1652	O N	LYS A	18	2.074	31.534	-14.713	1.00 1.00	190.00
	1653 1654	CA	LYS A	18	2.625	30.380	-15.402 -16.669	1.00	249.19
50	1655	CB	LYS A	18	1.798	30.115 28.904	-17.483	1.00	249.19
30	1656	CG	LYS A	18	2.212 1.206	28.655	-18.601	1.00	249.19
	1657	CD	LYS A	18 18	1.619	27.498	-19.493	1.00	249.19
	1658	CE	LYS A LYS A	18	2.837	27.814	-20.292	1.00	249.19 190.00
_	1659	NZ C	LYS A	18	4.101	30.602	-15.765 -16.368	1.00 1.00	190.00
5:	5 1660 1661	ŏ	LYS A	18	4.472	31.613	-15.390	1.00	217.86
	1662	Ñ	GLY A		4.945	29.648 29.759	-15.698		217.86
	1663	CA	GLY A		6.356 7.219	30.324	-14.582	1.00	217.86
_	1664	Ç	GLY A			30.261	-14.675		217.86 170.23
6	0 1665	0	GLY A GLU A			30.874	-13.537		170.23
	1666	N CA	GLU A		7.330	31.452	-12.399		186.84
	1667 1668	CB	GLU A	20	6.435	32.409	-11.611 -12.440		186.84
	1669	ČG	GLU A	20		33.418 34.410	-11.578		188.84
ϵ	55 1670	CD	GLU A			33.972	-10.688	1.00	186.84
	1671	OE1	GLU /				-11.79		186.84 170.23
	1672	OE2	GLU /	-		30.341	-11.450		170.23
	1673	C	GLU /		7.274	29.232	-11.46 -10.63		187.01
•	1674 70 1675	Ň	ASN			30,634	- 10.03		
	, 5 10/5	•							

1	678	CA	ASN A	21	9.372 10.888	29.622 29.456	-9.707 -9.859	1.00 1.00	187.01 249.69 249.69
	677	CB	ASN A	21	11.371	29.621	-11.291	1.00	249.69
	678	CG	ASN A	21 21	10.828	29.039	-12.233	1.00 1.00	249.69
1	679	OD1	ASN A	21	12.423	30.420	-11. 43 5 -8.230	1.00	187.01
	1680	ND2	ASN A	21	9.087	29.907	-7.786	1.00	187.01
	1681	C	ASN A	21	9.136	راد 28.842 28.842	-7.477	1.00	223.09
	1682 1683	Ň	VAL A	22	8.816	28.936	-6.050	1.00	223.09
	1684	CA	VAL A	22	8.516 6.995	28.809	-5.785	1.00	159.07 159.07
	1685	CB	VAL A	22 22	6.530	27.388	-6.039	1.00 1.00	159.07
	1686	CG1	VAL A VAL A	22	6.680	29.212	-4.363 - 200	1.00	223.09
	1687	CG2	VAL A	22	9.228	27.825	-5 280 -5 801	1.00	223.09
	1688	C	VAL A	22	9.418	26.731	-i 033	1.00	162.43
15	1689	N	THR A	23	9.600	28.102 27.125	-3.197	1.00	162.43
15	1690 1691	CA	THR A	23	10.307	27.680	-2.758	1.00	218.62 218.62
	1692	СВ	THR A	23 23	11.677 12.384	28.165	-3.905	1.00	218.62
	1693	OG1	THR A	23	12.498	26.594	-2.071	1.00 1.00	162.43
	1694	CG2	THR A THR A	23	9.549	26.715	-1.924 -1.114	1.00	162.43
20	1695	C	THR A	23	9.185	27.571	-1.736	1.00	159.52
	1696	O N	LEU A	24	9.337	25.410 24.916	-0.549	1.00	159.52
	1697	CA	LEU A	24	8.635	23.860	-0.923	1.00	128.43
	1698 1699	CB	LEU A	24	7.593 6.845	23.919	-2.252	1.00	128.43
25	1700	CG	LEU A	24	5.664	22.963	-2.175	1.00	128.43 128.43
2,5	1701	CD1	LEU A	24 24	6.352	25.322	-2.557	1.00 1.00	150.52
	1702	CD2	LEU A	24	9.600	24.299	0.464 0.247	1.00	159.52
	1703	C	LEU A	24	10.111	23.201	1,574	1.00	201.17
	1704	0 N	THR A	25	9.827	24.999 24.533	2.637	1.00	201.17
30	1705	ĞA	A FIHT	25	10.722	25.712	3.227	1.00	221.92
	1706 1707	CB	THR A	25		26.363	2.178	1.00	221.92 221.92
	1708	OG1	THR A	25		25.225	4.293	1.00	201.17
	1709	CG2	THR A	25 25		23.875	3.767	1.00 1.00	201.17
35	1710	Ç	THR A	25		24.429	4.215 4.232		178.89
	1711	O N	CYS A	26	10.363	22.707	5.311	_	178.89
	1712	CA	CYS A	26		21.995 22.556	6.672		178.89
	1713 1714	Č.	CYS A	26			6.885	1.00	178.89
40	1715	ŏ	CYS A	20		00 504	5.257		171.78 171.78
70	1716	CB	CYS A				6.366		234.74
	1717	SG	CYS A ASN A			22.623	7.589 8.929		234.74
	1718	N CA	ASN A		7 9.307		9.98	·	249.69
4.5	1719	CB	ASN A	. 2	7 8.59		11.35		249.69
45	1720 1721	ČĞ	ASN A		7 8.55		11.46	3 1.00	249.69
	1722	OD1	ASN A	٠.	27 8.19 27 8.92	T 4	12.39		2∔9.69 234.74
	1723	ND2	ASN A	-	27 8.92 27 10.77	2 23.362	9.32		234.74
	1724	C	ASN ASN	•	27 11.42	5 22.453	9.83 9.07		249.69
50	0 1725	O N			28 11.26	7 24.569	9.38	_	249.69
	1726	CA	GLY	Α :	28 12.64		8.70		249.69
	1727 1728	Č.	GLY	Α	28 12.8		7.5	51 1.00	249.69
	1729	ō	GLY		28 12.74 29 13.24	·	9.6		249.69 iə.69
5	5 1730	N	ASN	• •	29 13.2 29 13.4	00.044	9.1		249.69
	1731	CA	ASN ASN		29 13.4	₅₂ 29.617	^ 6		249.69
	1732	CB	ASN		29 13.4	₀₁ 31.093			249.69
	1733	CG OD1			29 13.2		40.0		249.69
	1734 50 1735	ND2			29 13.5		·	314 1.00	
•	1736	_	ASN		29 14.7	~ ~ ~		190 1.00	
	1737	_	ASN		29 14.7 30 15.8		5 8.8	B61 1.00	240.00
	1738	, N	ASN		30 15.0 30 17.	157 28.53	3 8.	158 1.00 895 1.00	
	1739	CA	ASN ASN			002 29.58	` _	895 1.00 911 1.00	040.00
1	65 1740			Â	30 17.	349 30.95	~	960 1.00	249.69
	1741					266 31.60 888 31.41		744 1.00	249.69
	1742 1743		2 ASN	I A			~ ~	.919 1.00	
	174	_	ASA			.985 27.26 .147 26.83		.774 1.0	249.69
	70 174		ASA	ı A	30 18				

						00.009	8.987	1.00	249.69
		N	PHE A	31	18.512	26.668 25.474	8.836	1.00	249.69
	746	CA	PHE A	31	19.345	25.733	9.416	1.00	249.69 249.69
	747 748	CB-	PHE A	31	20.748 21.429	26.957	8.841	1.00	249.69
	749	CG.	PHE A	31 31	21.106	28.234	9.300	1.00 1.00	249.69
	750	CD1	PHE A	31	22.372	26.835	7.822 8.749	1.00	249.69
	751	CD2	PHE A PHE A	31	21.706	29.372	7.263	1.00	249.69
	752	CE1 CE2	PHE A	31	22.978	27.971 29.238	7.730	1.00	249.69
	753	CZ	PHE A	31	22.644	24.200	9.450	1.00	249.69
10 1	754	Č	PHE A	31	18.752 18.444	24.144	10.647	1.00	249.69 249.69
	1755 1756	Ŏ	PHE A	31	18.608	23.175	8.608	1.00 1.00	249.69
	1757	N	PHE A	32 32	18.052	21.879	9.017	1.00	249.69
	1758	CA	PHE A PHE A	32	16.789	21.579	8.201 8.766	1.00	249.69
	1759	CB	PHE A	32	15.943	20.469	9.991	1.00	249.69
	1760	CG	PHE A	32	15.293	20.621 19.274	8.064	1.00	249.69
	1761	CD1 CD2	PHE A	32	15.785	19.598	10.509	1.00	249.69 249.69
	1762 1763	CE1	PHE A	32	14.496 14. 99 0	18.245	8.573	1.00	249.69
	1764	CE2	PHE A	32	14.345	18.408	9.798	1.00 1.00	249.69
20	1765	CZ	PHE A	32 32	19.088	20.757	8.821 8.170	1.00	249.69
20	1766	C	PHE A PHE A	32	20.125	20.964	9.358	1.00	231.29
	1767	0	GLU A	33	18.798	19.569	9.270	1.00	231.29
	1768	N CA	GLU A	33	19.741	18.455 18.036	10.688	1.00	249.69
25	1769	CB	GLU A	33	20.145	17.234	10.751	1.00	249.69 249.69
25	1770 1771	CG	GLU A	33	21.430 22.544	17.870	9.925	1.00	249.69
	1772	CD	GLU A	33	22.781	19.095	10.061	1.00 1.00	249.69
	1773	OE1	GLU A	33 33	23,193	17.142	9.140 8.477	1.00	231.29
	1774	OE2	GLU A	33	19.334	17.212	7.624	1.00	231.29
30	1775	C	GLU A	33	20.088	16.746	8.765	1.00	249.69
	1776	О N	VAL A	34	18.156	16.671 15.462	8.096	1.00	249.69
	1777	CA CA	VAL A	34	17.677	15.045	8.664	1.00	206.86 206.86
	1778 1779	CB	VAL A	34		13.765	8.012	1.00	206.86
35	1780	CG1	VAL A			14.858	10.166	1.00 1.00	249.69
"	1781	CG2	VAL A			15.536	6.560 5.977	1.00	249.69
	1782	Č	VAL A	` _	17.381	16.608	5.920		249.69
	1783	0	SER A		5 17.793	14.378 14.245	4.458	1.00	249.69
40	1784	N CA	SER A	∖ 3		13.478	3.941	1.00	177.13 177.13
40	1785	CB	SER A	, 3	5 18.968 5 18.874		4.268		249.69
	1786 1787	OG.	SER A			40.467	4.08		249.69
	1788	Ċ	SER	٠.	15 16.483 35 16.208	13.245	2.90		238.60
	1789	0	SER A		36 15.739	13.038	5.10 4.90	·	238.60
45	1790	N	SER		36 14.506		5.86	_	249.69
	1791	CA CB		Ä	36 14.43		7.20	ვ 1.00	249.69
	1792	og Og	SER	• •	36 14.20		5.12		238.60 238.60
	1793 1794	Č		• •	36 13.29 36 12.80	40.000	6.23	30 1.00	223.58
50) 1795	0		• •	36 12.80 37 12.83	₅ 13.795	4.00 4.00		223.58
٠,	1796	N	THR THR	• •	37 11.68	6 14.678	3.7		216.59
	1797	CA	THR	Â	37 12.10		4.7	23 1.00	216.59
	1798	CB QA1		Â	37 13.07		3.7	86 1.00	216.59
_	1799	ČG2		Α	37 10.90	44.400	3.0		223.58 223.58
5	5 1800 1801	Č	THR		37 10.76 37 11.1	40 773	1.9		040.60
	1802	Ō	THR		37 11.1° 38 9.4	44 440	3.3		0.40.00
	1803	N	LYS LYS		38 8.4	10 13.655		130 1.00 166 1.00	
	1804	CA	LYS	Â	38 7.4			770 1.00	249.69
6	50 1805	CB				32 11.473		515 1.00	
	1806	CG CD	LYS	. A		296 10.511 290 9.293	5.	053 1.00	
	1807 1808		LYS	3 A		060 9.293 181 8.326	; 5.	770 1.00	240.00
	1809		LYS	A		588 14.782	1.	806 1.00 456 1.0	- 40 00
	65 1810	C	LYS	5 A		301 15.793	, 2		0 201.19
,	1811	. 0	LY	S A P A	39 7.	229 14.61		.536 1.0 .171 1.0	0 201.19
	1812	. N		PA	39 6.	425 15.60	* .	.250 1.0	0 173.49
	1813			PA	39 7	256 16.29 384 17.17	· _	.741 1.0	
	1814	` ~		PA	39 8	.384 17.17	•		
	70 181	, •			•				

								4	
	1816	CD2	TRP A	39	8.282	18.328	0.122	1.00	173.49
	1817	CE2	TRP A	39	9.574	18.892	0.223	1.00	173.49
	1818	CE3	TRP A	39	7.223	18.950	0.812	1.00	173.49
				39	9.703	17.079	-1.099	1.00	173.49
_	1819	CD1					-0.528		
5	1820	NE1	TRP A	39	10.418	18.112		1.00	173.49
	1821	CZ2	TRP A	39	9.836	20.031	0.972	1.00	173.49
	1822	CZ3	TRP A	39	7.489	20.083	1.554	1.00	173.49
	1823	CH2	TRP A	39	8.785	20.611	1.629	1.00	173.49
			TRP A	39	5.263	14.870	-0.821	1.00	201.19
	1824	Ç					-1.463	1.00	
10	1825	0	TRP A	39	5.473	13.844			201.19
	1826	N	PHE A	40	4.045	15. 38 5	-0.655	1.00	233.06
	1827	CA	PHE A	40	2.875	14.733	-1.231	1.00	233.06
	1828	CB	PHE A	40	1.983	14.154	-0.122	1.00	249.42
						13.151	0.775	1.00	249.42
	1829	CG	PHE A	40	2.671				
15	1830	CD1	PHE A	40	3.484	13.580	1.820	1.00	249.42
	1831	CD2	PHE A	40	2.482	11.778	0.592	1.00	249.42
	1832	CE1	PHE A	40	4.098	12.658	2.674	1.00	249.42
		CE2	PHE A	40	3.089	10.854	1.435	1.00	249.42
	1833					11.294	2.479	1.00	249.42
	1834	CZ	PHE A	40	3.899				
20	1835	С	PHE A	40	2.023	15.621	-2.139	1.00	233.06
	1836	0	PHE A	40	0.945	16.063	-1.744	1.00	233.06
	1837	N	HIS A	41	2.506	15.858	-3.358	1.00	146.58
		CA	HIS A	41	1.787	16.676	-4.340	1.00	146.58
	1838				2.663		-5.569	1.00	196.00
	1839	CB	HIS A	41		16.905			
25	1840	CG	HIS A	41	2.012	17.747	-6.619	1.00	196.00
	1841	CD2	HIS A	41	2.035	17.661	-7.971	1.00	196.00
	1842	ND1	HIS A	41	1.259	18.864	-6.322	1.00	196.00
		CE1	HIS A	41	0.849	19.429	-7.441	1.00	196.00
	1843						-8.457	1.00	196.00
	1844	NE2	HIS A	41	1.308	18.719			
30	1845	С	HIS A	41	0.459	16.041	-4.776	1.00	146.58
	1846	0	HIS A	41	0.458	15.095	-5.564	1.00	146.58
	1847	Ň	ASN A	42	-0.660	16.586	-4.280	1.00	208.40
		CA	ASN A	42	-2.004	16.067	-4.570	1.00	208.40
	1848						-6.087	1.00	249.69
	1849	CB	ASN A	42	-2.229	15.933			
35	1850	CG	ASN A	42	-2.538	17.270	-6. 763	1.00	249.69
	1851	OD1	ASN A	42	-1.824	18.251	-6.553	1.00	249.69
	1852	ND2	ASN A	42	-3.591	17.305	-7.583	1.00	249.69
			ASN A	42	-2.173	14,703	-3.887	1.00	208.40
	1853	C					-4.302	1.00	208.40
	1854	0	ASN A	42	-2.981	13.871			
40	1855	N	GLY A	43	-1.401	14.499	-2.824	1.00	249.69
	1856	CA	GLY A	43	-1.445	13.248	-2.092	1.00	249.69
	1857	C	GLY A	43	-0.354	12.288	-2.55 5	1.00	249.69
		ŏ	GLY A	43	0.302	11.620	-1.744	1.00	249.69
	1858						-3.870	1.00	243.81
	1859	N	SER A	44	-0.158	12.222			
45	4860	CA	SER A	44	0.845	11.350	-4.481	1.00	243.81
	1861	CB	SER A	44	0.812	11.493	-6.004	1.00	249.09
	1862	ÖĞ	SER A	44	-0.450	11.141	-6.535	1.00	249.69
				44	2.250	11.676	-4.002	1.00	243.81
	1863	C	SER A						243.81
	1864	0	SER A	44	2.714	12.806	-4.162	1.00	
50	1865	N	LEU A	45	2.936	10.687	-3.437	1.00	249.69
	1866	CA	LEU A	45	4.294	10.912	-2.958	1.00	249.69
	1867	СВ	LEU A	45	4.913	9.605	-2.458	1.00	240.25
				45	6.324	9.745	-1.879	1.00	240.25
	1868	CG							240.25
	1069	CD1	LEU A	45	6.328	10.787	-0.773	1.00	
55	1870	CD2	LEU A	45	6.798	8.405	-1.351	1.00	240.25
	1871	С	LEU A	45	5.160	11.512	-4.070	1.00	249.09
	1872	Õ	LEU A	45	4.939	11.248	-5.256	1.00	249.69
			SER A	46	6.136	12.329	-3.675	1.00	216.07
	1873	N						1.00	216.07
	1874	CA	SER A	46	7.028	12.988	-4.621		
60	1875	СВ	SER A	46	7.156	14.473	-4.270	1.00	249.69
	1876	OG	SER A	46	7.934	15.159	-5.237	1.00	249.69
		Č	SER A	46	8.409	12.344	-4.645	1.00	216.07
	1877					11.515	-3.795	1.00	216.07
	1878	0	SER A	46	8.733			1.00	
	1879	N	GLU A	47	9.223	12.753	-5.616	1.00	204.74
65	1880	CA	GLU A	47	10.572	12.214	-5.797	1.00	204.74
	1881	CB	GLU A	47	10.901	12.162	-7.289	1.00	249.69
		ČĠ	GLU A	47	9.973	11.256	-8.078	1.00	249.69
	1882					11.239	-9.554	1.00	249.69
	1883	CD	GLU A	47	10.299				
	1884	OE1	GLU A	47	10.185	12.307	-10.203	1.00	249.69
70	1885	OE2	GLU A	47	10.673	ļ0.15 8	-10.066	1.00	249.69

	1886	С	GLU A	47	11.702	12.933	-5.059	1.00	204.74
	1887	0	GLU A	47	12.819	12.424	-4.995	1.00	204.74 204.74
	1888	N	GLU A		11.429	14.113	-4.512	1.00	206.77
5	1889 1890	CA CB	GLU A		12.459 12.206	14.833 16.344	-3.780 -3.813	1.00	206.77
	1891	CG	GLU A		13.200	17.159	-3.812 -2.982	1.00 1.00	249.43
	1892	CD	GLU A	48	14.627	17.087	-3.507	1.00	249.43 249.43
	1893	OE1	GLU A		14.902	17.685	-4.569	1.00	249.43
10	1894 1895	OE2 C	GLU A		15.472 12.492	16.431 14.344	-2.859	1.00	249.43
••	1896	ŏ	GLU A		11.500	13.825	-2.335 -1.811	1.00 1.00	206.77
	1897	N	THR A	49	13.648	14.506	-1.702	1.00	206.77 249.69
	1898	CA	THR A		13.844	14.085	-0.324	1.00	249.69
15	1899 1900	CB OG1	THR A		14.806	12.890	-0.252	1.00	249.53
13	1901	CG2	THR A		16.030 14.174	13.218 11.671	-0.928 -0.909	1.00	249.53
	1902	c	THR A		14.417	15.232	0.500	1.00 1.00	249.53 249.69
	1903	0	THR A	49	14.224	15.294	1.716	1.00	249.69
20	1904	N	ASN A		15.128	16.136	-0.166	1.00	249.69
20	1905 1906	CA CB	ASN A		15.710 16.438	17.294	0.504	1.00	249.69
	1907	CG	ASN A		17.276	18.174 19.254	-0.519 0.134	1.00 1.00	232.42
	1908	OD1	ASN A	50	17.063	19.590	1.301	1.00	232.42 232.42
25	1909	ND2	ASN A		18.219	19.813	-0.615	1.00	232.42
23	1910 1911	C	ASN A		14.552	18.073	1.142	1.00	249.69
	1912	N	SER A		13.423 14.817	18.003 18.808	0.658 2.217	1.00	249.69
	1913	CA	SER A		13.759	19.568	2.873	1.00 1.00	181.87 181.87
20	1914	CB	SER A	51	14.240	20.110	4.220	1.00	249.47
30	1915	og	SER A		15.152	21.181	4.047	1.00	249.47
	1916 1917	C	SER A		13.249	20.725	2.016	1.00	181.87
	1918	Ň	SER A		12.180 14.007	21.269 21.104	2.293 0.984	1.00 1.00	181.87
~~	1919	CA	SER A	52	13.606	22.199	0.087	1.00	193.91 193.91
35	1920	CB	SER A		14.735	23.217	-0.086	1.00	144.08
	1921 1922	og	SER A		15.064	23.831	1.139	1.00	144.08
	1923	C	SER A		13.196 14.045	21.706 21.367	-1.297 -2.126	1.00	193.91
	1924	Ň	LEU A		11.890	21.680	-1.539	1.00 1.00	193.91 177.42
40	1925	CA	LEU A		11.346	21.239	-2.817	1.00	177.42
	1926	CB	LEU A		10.034	20.488	-2.595	1.00	145.45
	1927 1928	CG CD1	LEU A	53 53	9.082 9.821	20.340	-3.785	1.00	145.45
	1929	CD2	LEU A		7.997	19.891 19.343	-5.043 -3.401	1.00 1.00	145.45 145.45
45	1930	C	LEU A	53	11.108	22.423	-3. 73 7	1.00	177.42
	1931	0	LEU A		10.143	23.168	-3.574	1.00	177.42
	1932 1933	N CA	ASN A	54 54	11.991	22.591	-4.709	1.00	220.39
	1934	CB	ASN A	54 54	11.845 13.187	23.692 24.045	-5. 63 5 -6.254	1.00 1.00	220.39
50	1935	CG	ASN A	54	14.109	24.677	-5.264	1.00	193.36 193.36
	1936	OD1	ASN A		13.746	25.644	-4.602	1.00	193.36
	1937 1938	ND2	ASN A	54	15.311	24.140	-5.145	1.00	193.36
	1939	C O	ASN A ASN A		10.834 10.486	23.415 22.267	-6.729 -7.000	1.00	220.39
55	1940	Ň	ILE A		10.362	24.496	-7.009 -7.333	1.00 1.00	220.39 206.48
	1941	CA	ILE A		9.393	24.451	-8.415	1.00	206.48
	1942	CB	ILE A		7.984	24.867	-7.921	1.00	168.43
	1943 1944	CG2 CG1	ILE A		7.135	25.353	-9.080	1.00	168.43
60	1945	CD1	ILE A		7.316 5.920	23.696 24.004	-7.206 -6.681	1.00 1.00	168.43
	1946	C	ILE A		9.877	25.442	-9.459	1.00	168.43 206.48
	1947	0	ILE A	55	9.979	26.641	-9.190	1.00	206.48
	1948	N CA	VAL A		10.194	24.943	-10.646	1.00	242.77
65	1949 1950	CA CB	VAL A		10.667	25.821 25.165	-11.700	1.00	242.77
	1951	CG1	VAL A		11.790 12.589	25.165 26.233	-12.499 -13.240	1.00 1.00	249.69 249.69
	1952	CG2	VAL A	56	12.687	24.377	-11.562	1.00	249.69 249.69
	1953	Ç	VAL A	56	9.511	26.168	-12.624	1.00	242.77
70	1954 1955	O N	VAL A		8.354	26.060	-12.225	1.00	242.77
, ,	1000	14	ASN A	57	9.822	26.580	-13.853	1.00	177.18

1	1956 1957 1958	CA CB CG.	ASN A	57 57 57 57	8.804 9.265 10.430 10.372	26.971 26.619 27.489 28.721	-14.835 -16.250 -16.705 -16.617 -17.187	1.00 1.00 1.00 1.00 1.00	177.18 249.69 249.69 249.69 249.69
5	1959 1960 1961 1962	OD1' ND2 C O	ASN A ASN A	57 57 57	11.494 7.436 7.105 6.661	26.853 26.374 25.264 27.166	-14.547 -14.964 -13.816	1.00 1.00 1.00	177.18 177.18 241.59
	1963 1964 1965 1966	N CA CB C	ALA A ALA A ALA A	58 58 58 58 58	5.322 4.739 4.339 3.857	26.838 28.038 26.363 27.134	-13.362 -12.623 -14.416 -15.237	1.00 1.00 1.00 1.00	241.59 177.10 241.59 241.59 126.26
15	1967 1968 1969 1970	O N CA CB	ALA A LYS A LYS A LYS A	59 59 59	4.031 3.078 3.620	25.077 24.446 23.088 23.183	-14.363 -15.277 -15.761 -16.494	1.00 1.00 1.00 1.00	126.26 249.69 249.69
13	1971 1972 1973	CG CD CE NZ	LYS A LYS A LYS A LYS A	59 59 59 59	4.959 5.515 6.883 7.458	21.808 21.939 20.619 24.246	-16.859 -17.528 -17.910 -14.486	1.00 1.00 1.00 1.00	249.69 249.69 249.69 126.26
20	1974 1975 1976 1977	C O N CA	LYS A LYS A PHE A PHE A	59 59 60 60	1.790 1.810 0.672 -0.622	23.891 24.490 24.356	-13.311 -15.139 -14.497 -15.570	1.00 1.00 1.00 1.00	126.26 178.77 178.77 238.68
25	1978 1979 1980 1981	CB CG CD1 CD2	PHE A PHE A PHE A PHE A	60 60 60	-1.715 -1.824 -2.296 -1.468	24.325 25.601 25.585 26.820	-16.362 -17.670 -15.794 -18.400	1.00 1.00 1.00 1.00	238.68 238.68 238.68 238.68
30	1982 1983 1984 1985	CE1 CE2 CZ C	PHE A PHE A PHE A PHE A	60 60 60	-2.411 -1.580 -2.053 -0.746	26.758 28.002 27.969 23.132	-16.515 -17.821 -13.592 -12.588	1.00 1.00 1.00 1.00	238.68 238.68 178.77 178.77
	1986 1987 1988 1989	O N CA	PHE A GLU A GLU A GLU A	60 61 61 61	-1.468 -0.040 -0.076 0.665	23.162 22.063 20.822 19.719	-13.948 -13.181 -13.945 -15.330	1.00 1.00 1.00 1.00	249.03 249.03 249.30 249.30
35	1990 1991 1992 1993	CB CG CD OE1	GLU A GLU A GLU A GLU A	61 61 61 61	0.091 0.076 1.132 -0.997	19.402 20.605 21.254 20.895	-16.264 -16.436 -16.833	1.00 1.00 1.00	249.30 249.30 249.30 249.03
40	1994 1995 1996 1997	OE2 C O N	GLU A GLU A ASP A	61 61 62 62	0.537 0.222 1.412 2.062	20.991 20.236 21.984 22.251	-11.792 -10.870 -11.648 -10.372	1.00 1.00 1.00 1.00	249.03 157.91 157.91 172.18
45	2001	CA CB CG OD1	ASP A ASP A ASP A ASP A	62 62 62 62	3.191 4.167 4.368	23.264 22.856 21.633 23.753	-10.539 -11.598 -11.779 -12.244		172.18 172.18 172.18 172.18 157.91
50	2002 2003 2004) 2005	OD2 C O . N	ASP A ASP A SER A SER A	62 2 63	1.058 1.266 -0.026	22.795 22.700 23.384 23.933	-9.366 -8.159 -9.864 -8.991	1.00 1.00 1.00	157.91 191.12 191.12 203.60
	2006 2007 2008 2009	CA CB OG C	SER A SER A SER A	63 63 63	-2.179 -1.685 -1.634	24.576 25.593 22.778 21.773	-9.822 -10.67 -8.18 -8.75	1.00 6 1.00 3 1.00	203.60 191.12 191.12 195.42
5	5 2010 2011 2012 2013	O N CA C	SER A GLY A GLY A	64 64 A 64 A 64	4 -1.662 4 -2.199 4 -1.967	22.907 21.821 21.897 22.940	-6.87 -6.08 -4.59 -4.06	7 1.00 6 1.00 9 1.00	195.42 195.42 195.42 249.69
6	2014 2015 2016 2017	O N CA CB	GLU A GLU A	A 6 A 6	5 -2.199 5 -2.064 5 -3.302 5 -3.277	19.876	-3.93 -2.46 -1.96 -0.5	1.00 14 1.00	249.69 246.11 246.11 246.11
(2018 2019 65 2020 2021	CG CD OE1 OE2 C		A 6 A 6	55 -4.310 65 -4.201 65 -5.230 65 -0.790	18.417 17.309 18.684 19.844	-0.26 -0.7 0.5 -2.1 -2.5	79 1.00 97 1.00 12 1.00	246.11 246.11 249.69 249.69
	2022 2023 2024 70 2025	. O	GLU TYR TYR	A	65 -0.613 66 0.083 66 1.33	3 20.456	-2.5 -1.3 -0.8	08 1.00	400 07

	2026	СВ	TYR A	ec	0.504	00.044			
	2027	CG	TYR A	66 66	2.534 2.737	20.641 20.798	-1.324 -2.807	1.00	181.47
	2028	CD1	TYR A	66	1.966	21.687	-3.549	1.00 1.00	181.47 181.47
5	2029	CE1	TYR A	66	2.227	21.911	-4.896	1.00	181.47
3	2030 2031	CD2 CE2	TYR A	66	3.769	20.122	-3.454	1.00	181.47
	2032	CZ	TYR A TYR A	66 66	4.040 3.2 6 8	20.332	-4.800	1.00	181.47
	2033	OH	TYR A	66	3.561	21.230 21.460	-5.513 -6.838	1.00	181.47
	2034	C	TYR A	66	1.462	19.616	0.622	1.00 1.00	181.47
10	2035	0	TYR A	66	0.665	20.149	1.402	1.00	196.27 196.27
	2036	N	LYS A	67	2.493	18.862	1.021	1.00	214.47
	2037 2038	CA CB	LYS A LYS A	67 67	2.778	18.572	2.435	1.00	214.47
	2039	CG	LYS A	67 67	1.630 1.262	17.783 16.527	3.059	1.00	179.29
15	2040	CD	LYS A	67	0.071	15.859	2.300 2.955	1.00 1.00	179.29
	2041	CE	LYS A	67	-0.626	14.887	2.008	1.00	179.29 179.29
	2042	NZ	LYS A	67	-1.808	14.194	2.632	1.00	179.29
	2043 2044	C	LYS A	67	4.077	17.799	2.681	1.00	214.47
20	2045	O N	LYS A CYS A	67 68	4.546	17.060	1.826	1.00	214.47
	2046	CA	CYS A	68	4.644 5.865	17.981 17.291	3.869	1.00	202.66
	2047	C	CYS A	68	5.713	16.618	4.259 5.621	1.00 1.00	202.66
	2048	0	CYS A	68	4.961	17.075	6.483	1.00	202.66 202.66
25	2049	СВ	CYS A	68	7.067	18.245	4.273	1.00	195.74
23	2050	SG	CYS A	68	7.101	19.551	5.556	1.00	195.74
	2051 2052	N CA	GLN A GLN A	69	6.439	15.519	5.797	1.00	233.18
	2053	CB	GLN A	69 69	6.420 5.367	14.730	7.024	1.00	233.18
	2054	ČĠ	GLN A	69	5.562	13.631 12.460	6.896 7.835	1.00 1.00	249.69
30	2055	CD	GLN A	69	4.580	11.333	7.569	1.00	249.69 249.69
	2056	OE1	GLN A	69	4.451	10.865	6.436	1.00	249.69
	2057	NE2	GLN A	69	3.888	10.885	8.615	1.00	249.69
	2058 2059	C	GLN A GLN A	69	7.798	14.111	7.224	1.00	233.18
35	2060	Ň	GLN A HIS A	69 70	8.485 8.206	13.796 13.942	6.254	1.00	233.18
-	2061	ĊA	HIS A	70 70	9.508	13.348	8.477 8.757	1.00 1.00	249.54
	2062	CB	HIS A	70	10.202	14.086	9.904	1.00	249.54 249.69
	2063	CG	HIS A	70	10.674	15.458	9.536	1.00	249.69
40	2064 2065	CD2	HIS A	70	10.459	16.662	10.116	1.00	249.69
₩	2066	ND1 CE1	HIS A HIS A	70 70	11.475	15.699	8.439	1.00	249.69
	2067	NE2	HIS A	70 70	11.731 11.126	16.992 17.600	8.359	1.00	249.69
	2068	Ċ	HIS A	70	9.393	11.867	9.366 9.084	1.00 1.00	249.69 249.54
4.5	2069	0	HIS A	70	8.327	11.270	8.917	1.00	249.54
45	2070	N	GLN A	71	10.496	11.283	9.549	1.00	249.69
	2071 2072	CA CB	GLN A GLN A	71	10.546	9.863	9.894	1.00	249.69
	2072	CG	GLN A GLN A	71 71	11.944	9.520	10.429	1.00	249.69
	2074	CD	GLN A	71	12.318 12.356	8.033 7.432	10.415 9.015	1.00	249.69
50	2075	OE1	GLN A	71	12.933	8.009	8.090	1.00 1.00	249.69 249.69
	2076	NE2	GLN A	71	11.749	6.257	8.859	1.00	249.69
	2077	C	GLN A	71	9.474	9.485	10.925	1.00	249.69
	2078 2079	O	GLN A	71	8.737	8.505	10.747	1.00	249.69
55	2080	N CA	GLN A GLN A	72 72	9.383	10.270	11.995	1.00	249.69
	2081	CB	GLN A	72 72	8.413 9.148	10.013 9.484	13.056	1.00	249.69
	2082	CG	GLN A	72	8.266	9.132	14.292 15.487	1.00 1.00	249.69 249.69
	2083	CD	GLN A	72	9.085	8.768	16.717	1.00	249.69
60	2084	OE1	GLN A	72	9.910	7.853	16.679	1.00	249.69
OU	2085	NE2	GLN A	72	8.860	9.486	17.817	1.00	249.69
	2086 2087	C	GLN A GLN A	72 72	7.634	11.288	13.402	1.00	249.69
	2088	N	VAL A	72 73	7.602 7.011	11.722	14.558	1.00	249.69
	2089	CA	VAL A	73 73	6.233	11.891 13.108	12.393 12.595	1.00	249.69
65	2090	CB	VAL A	73	7.036	14.377	12.393	1.00 1.00	249.69 239.35
	2091	CG1	VAL A	73	6.321	15.615	12.720	1.00	239.35
	2092	CG2	VAL A	73	8.449	14.304	12.750	1.00	239.35
	2093 2094	CO	VAL A	73 72	4.979	13.047	11.731	1.00	249.69
70	2095	N	VAL A ASN A	73 74	5.014 3.875	12.526	10.619	1.00	249.69
		• •	7011 7	• •	3.0/5	13.578	12.245	1.00	249.69

					0.607	13.580	11.494	1.00	249.69
	2096	CA	, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	• •	2.627 1.448	13.799	12.450	1.00	244.75
	2097	CB		74 74	1.421	12.775	13.581	1.00	244.75
	2098	CG	ASN A	74 74	1.672	11.588	13.354	1.00	244.75
	2099	OD1	ASN A ASN A	74	1.112	13.230	14.793	1.00	244.75 249.69
5	2100	ND2	ASN A	74	2.667	14.663	10.404	1.00 1.00	249.69 249.69
	2101	C	ASN A	74	2.979	15.828	10.680 9.167	1.00	249.69
	2102	Ň	GLU A	75	2.362	14.262	8.008	1.00	249.69
	2103 2104	ČA	GLU A	75	2.370	15.160 14.485	6.826	1.00	249.69
10	2104	СВ	GLU A	75	1.656	13.641	7.216	1.00	249.69
10	2106	CG	GLU A	75	0.447 -0.086	12.806	6.064	1.00	249.69
	2107	CD	GLU A	75 75	0.722	12.115	5.408	1.00	249.69
	2108	OE1	GLU A	75 75	-1.312	12.831	5.820	1.00	249.69
_	2109	OE2	GLU A GLU A	75 75	1.786	16.556	8.262	1.00	249.69 249.69
15	2110	C	GLU A	75	0.776	16.714	8.954	1.00 1.00	249.69
	2111	0 N	SER A	76	2.437	17.562	7.682 7.833	1.00	249.69
	2112	CA	SER A	76	2.037	18.959	7.212	1.00	185.73
	2113 2114	CB	SER A	76	3.093	19.877 19.838	5.796	1.00	185.73
20	2115	OG	SER A	76	3.026	19.291	7.206	1.00	249.69
20	2116	С	SER A	76 76	0.691 0.212	18.589	6.316	1.00	249.69
	2117	0	SER A	76 77	0.212	20.382	7.677	1.00	249.69
	2118	N _.	GLU A GLU A	77 77	-1.187	20.845	7.153	1.00	249.69 249.63
	2119	CA	GLU A	77	-1.695	22.053	7.952	1.00	249.63
25	2120	CB	GLU A	77	-2.038	21.734	9.394	1.00 1.00	249.63
	2121	CD	GLU A	77	-3.175	20.742	9.515 8.477	1.00	249.63
	2122	OE1	GLU A	77	-3.606	20.194	10.653	1.00	249.63
	2123 2124	OE2	GLU A	77	-3.633	20.508 21.250	5.701	1.00	249.69
30	2125	Č_	GLU A	77	-0.961	22,226	5,423	1.00	249.69
50	2126	Ò	GLU A	77	-0.262 -1.556	20.502	4.757	1.00	227.00
	2127	N	PRO A	78 78	-1.550 -2.599	19.491	4.999	1.00	247.88
	2128	CD	PRO A	78	-1.413	20.781	3.321	1.00	227.00 247.88
	2129	CA	PRO A PRO A	78	-2.583	20.012	2.710	1.00 1.00	247.88
35		CB CG	PRO A	78	-2.752	18.854	3.641 2.998	1.00	227.00
	2131	C	PRO A	78	-1.488	22.271	3.771	1.00	227.00
	2132 2133	ŏ	PRO A	78	-2.039	23.054 22.665	1.871	1.00	169.93
	2134	Ň	VAL A	79	-0.910	24.059	1.435	1.00	169.93
40		CA	VAL A	79	-0.966 0.390	24.785	1.549	1.00	154.03
-10	2136	СВ	VAL. A	79 79	0.329	26.125	0.825	1.00	154.03 154.03
	2137	CG1	VAL A VAL A	79	0.721	25.022	3.014	1.00	169.93
	2138	CG2	VAL A	79	-1.342	23.987	-0.017 -0.710	1.00 1.00	169.93
44	2139	C	VAL A	79	-0.883	23.087	-0.710	1.00	161.75
4.	5 2140 2141	Ň	TYR A	80	-2.175	24.911 24.874	-1.888	1.00	161.75
	2142	ĊA	TYR A	80	-2.581	25.028	-2.025	1.00	221.72
	2143	СВ	TYR A	80	-4.096 -4.606	24,573	-3.372	1.00	221.72
	2144	CG	TYR A	80 80	-4.874	23.227	-3.618	1.00	221.72
5	0 2145	CD1	TYR A	80	-5.296	22.792	-4.874		221.72 221.72
	2146	CE1	TYR A TYR A	80	-4.773	25.478	-4.418		221.72
	2147	CD2 CE2	TYR A		-5.193	25.052	-5.679 -5.896		221.72
	2148	CZ	TYR A		-5.451	23.708	-7.134		221.72
-	2149 5 2150	OH	TYR A	80	-5.860	23.276 25.939	-2.725		161.75
	2151	C	TYR A		-1.895	27.096	-2.329		161.75
	2152	0	TYR A		-1.812 -1.405	25.534	-3.889		159.92
	2153	N	LEU A			26.451	-4.78		159.92 117.26
	2154	CA	LEU A			25.951	-5.13		117.26
(50 2155	CB	LEU A	-	1,353	26.823	-6.18		117.26
	2156	CG CD1	LEU A		1.556	28.213	-5.60 -6.60		117.26
	2157	CD2	LEU /	A 81	2.692	26.221	-6.06		159.92
	2158 2159	C	LEU /	A 81	-1.550	26.562 25.541	-6.67		159.92
	65 2160	ŏ	LEU /	A 81		27.786	-6.47		176.90
	2161	N	GLU A			27.978	-7.70	9 1.00	176.90
	2162	CA	GLU A			28.697	-7.42		239.33
	2163	CB	GLU GLU	• •		28.382	-8.4		239.33 239.33
	2164	CG	GLU	A 8		29.072	-8.10	66 1.00	203.00
	70 2165	CO	323						

	2166 2167	OE1 OE2	GLU A	82 82	-6.678 -7.038	29.235 29.437 28.772	-6.970 -9.139 -8.720	1.00 1.00 1.00	239.33 239.33 176.90
	2168	C ·	GLU A	82	-1.815	29.768	-8.369	1.00	176.90
	2169	0	GLU A	82	-1.176 -1.818	28.315	-9.973	1.00	167.08
5 ,	2170	N	VAL A	83 83	-1.078	28.988	<i>-</i> 11.050	1.00	167.08
- ,	2171	CA	VAL A VAL A	83	-0.163	28.034	-11.817	1.00	127.07
	2172	CB	VAL A VAL A	83	0.595	28.807	-12.899	1.00	127.07
	2173	CG1	VAL A	83	0.800	27.368	-10.847	1.00	127.07 167.08
	2174	CG2	VAL A	83	-2.036	29.634	-12.043	1.00 1.00	167.08
10	2175	C O	VAL A	83	-3.077	29.071	-12.390 -12.524	1.00	136.71
	2176 2177	Ň	PHE A	84	-1.653	30.810	-13.412	1.00	136.71
	2178	ČA	PHE A	84	-2.502	31.588 32.805	-12.669	1.00	180.02
	2179	CB	PHE A	84	-3.039	32.481	-11.481	1.00	180.02
15	2180	CG	PHE A	84	-3.878	32.143	-10.263	1.00	180.02
	2181	CD1	PHE A	84	-3.296 -5.259	32.534	-11.575	1.00	180.02
	2182	CD2	PHE A	84 84	-4.085	31.871	-9.157	1.00	180.02
	2183	CE,	PHE A PHE A	84	-6.055	32.266	-10.484	1.00	180.02 180.02
	2184	CE2	PHE A	84	-5.471	31.933	-9.274	1.00	136.71
20	2185	CZ C	PHE A	84	-1.917	32.125	-14.692	1.00 1.00	136.71
	2186	ŏ	PHE A	84	-0.710	32.289	-14.838	1.00	185.25
	2187	Ň	SER A	85	-2.822	32.440	-15.606 -16.871	1.00	185.25
	2188 2189	ČA	SER A	85	-2.470	33.050	-18.036	1.00	191.52
25	2190	CB	SER A	85	-2.639	32.088 32.736	-19.246	1.00	191.52
23	2191	OG	SER A	85	-2.269	34.193	-17.012	1.00	185.25
	2192	С	SER A	85	-3.462 -4.680	33.960	-17.105	1.00	185.25
	2193	0	SER A	85 86	-4.660 -2.940	35.422	-17.002	1.00	167.09
	2194	N	ASP A	86 86	-3.769	36.623	-17.117	1.00	167.09
30	2195	CA	ASP A ASP A	86	-4.744	36.701	-15.951	1.00	156.75 156.75
	2196	CB	ASP A	86	-6.072	37.252	-16.358	1.00	156.75
	2197	CG OD1	ASP A	86	-6.110	38.341	-16.985	1.00 1.00	156.75
	2198	OD2	ASP A	86	-7.083	36.587	-16.045 -17.101	1.00	167.09
35	2199 2200	C	ASP A	86	-2.888	37.852	-16.775	1.00	167.09
33	2201	ŏ	ASP A	86	-1.708	37.760 39.005	-17.438	1.00	147.13
	2202	N	TRP A	87	-3.455	40.233	-17.435	1.00	147.13
	2203	CA	TRP A	87	-2.665 -3.446	41.371	-18.079	1.00	200.84
	2204	CB	TRP A	87	-3. 440 -3.221	41.441	-19.553	1.00	200.84
40	2205	CG	TRP A	87 87	-4.022	40.824	-20.563	1.00	200.84
	2206	CD2	TRP A	87	-3.413	41.103	-21.798	1.00	200.84 200.84
	2207	CE2 CE3	TRP A	87	-5.199	40.061	-20.542	1.00 1.00	200.84
	2208	CD1	TRP A	87	-2.185	42.053	-20.202	1.00	200.84
45	2209 2210	NE1	TRP A	87	-2.292	41.854	-21.551 -23.002	1.00	200.84
43	2211	CZ2	TRP A	87	-3.942	40.645 39.602	-21.752	1.00	200.84
	2212	CZ3	TRP A	87	-5.726	39.899	-22.961	1.00	200.84
	2213	CH2	TRP A	87	-5.095 -2.233	40.608	-16.017	1.00	147.13
	2214	C	TRP A	87 87	-1.040	40.785	-15.743	1.00	147.13
50	2215	0	TRP A LEU A	88	-3.198	40.715	-15.108	1.00	135.82 135.82
	2216	N	LEU A		-2.886	41.049	-13.725	1.00	139.19
	2217	CA	LEU A		- 400	42.416	-13.368	1.00 1.00	139.19
	2218	CB CG	LEU A	88	-2.870	43.605	-14.1 11 -13.593		139.19
5:	2219 5 2220	CD1	LEU			44.912	-14.008		139.19
Э.	2221	CD2	LEU A	. 88		43.608	-12.772		135.82
	2222	C	LEU A			39.996 39.439	-12.976		135.82
	2223	Ó	LEU A			39.710	-11.736		146.34
	2224	N	LEU A			38.737	-10.728		146.34
6	0 2225	CA	LEU A			37.466	-10.826	1.00	125.53 125.53
	2226	CB	LEU /	-		36.431	-9.74		125.53
	2227	CG	LEU /	-		38.143	-9.71		125.53
	2228	CD1	LEU	-		35.168	-10.00		146.34
,	2229	CD2 C	LEU	-	9 -2.854	39.355	-9.35 -9.07		146.34
C	55 2230 2231	ŏ	LEU		9 -1.785	39.903	-9.07 -8.50		124.61
	2231	Ň	LEU	A 8	0 -3.875	39.282	-6.50 -7.17		124.61
	2232	CA	LEU	A 8	0 -3.762		-6.68		89.03
	2234	СВ	LEU	Ă Ş	90 -5.132 90 -5.136		-5.23		89.03
•	70 2235	ca	LEU.	A 1	90 -5.136				

						-5.091	1.00	89.03
0000	CD1			1.192	41.932 41.132	-4.782	1.00	89.03
2236 2237	CD2			6.549	38.861	-6.196	1.00	124.61
2237	C			3.160	37.842	-5.902	1.00	124.61
2239	o ·			3.766 1.972	39.147	-5.686	1.00	143.99
5 2240	N	GG		1.335	38.229	-4.757	1.00	143.99
2241	CA			0.139	38.062	-5.110	1.00	163.37 163.37
2242	CB			0.382	37.527	-6.497	1.00 1.00	163.37
2243	CG		91	1.861	37.383	-6.798 -6.721	1.00	163.37
2244	CD OE1	GLN A	91	2.620	38.356	-0.721 -7.143	1.00	163.37
10 2245	NE2	GLN A	91	2.283	36.166	-3.304	1.00	143.99
2246 2247	C	GLN A	••	-1.463	38.676 39.872	-2.991	1.00	143.99
2248	ŏ	GLN A		-1.322	37.706	-2.421	1.00	122.21
2249	N	ALA A	92	-1.725 -1.862	37.978	-0.991	1.00	122.21
15 2250	CA	ALA A	92 92	-3.283	37.702	-0.548	1.00	218.43 122.21
2251	СВ	ALA A ALA A	92	-0.892	37.128	-0.190	1.00 1.00	122.21
2252	C	ALA A	92	-0.653	35.960	-0.527 0.861	1.00	143.19
2253	0 N	SER A	93	-0.338	37.733	1.742	1.00	143.19
2254	CA	SER A	93	0.612	37.067 37.975	2.935	1.00	121.60
20 2255 2256 \	CB	SER A	93	0.964	38.446	3.608	1.00	121.60
2257	OG	SER A	93	-0.192	35.790	2.220	1.00	143.19
2258	С	SER A	93	-0.030 0.452	34.690	1.941	1.00	143.19
ي 2259	0	SER A	93 94	-1.121	35.958	2.948	1.00	129.43 129.43
25 2260	N _.	ALA A ALA A	94	-1.880	34.831	3.446	1.00 1.00	204.58
2261	CA	ALA A	94	-1.688	34.686	4.950	1.00	129.43
2262	CB	ALA A	94	-3.322	35.190	3.108 2. 96 9	1.00	129.43
2263	C	ALA A	94	-3.620	36.387	2.955	1.00	144.02
2264	N	GLU A	95	-4.208	34.193 34.499	2.632	1.00	144.02
30 2265 2266	CA	GLU A	95	-5.601	33.467	1.668	1.00	173.81
2267	СВ	GLU A	95	-6.144 -5. 43 4	33.492	0.344	1.00	173.81
2268	CG	GLU A	95 95	-6.123	32.642	-0.695	1.00	173.81 173.81
2269	CD	GLU A	95	-5.590	32.539	-1.831	1,00 1.00	173.81
35 2270	OE1	GLU A	95	-7.201	32.078	-0.378 3.879	1.00	144.02
2271	OE2 C	GLU A	95	-6.488	34.587	3.857	1.00	144.02
2272	ŏ	GLU A	95	-7.548	35.222 33.951	4.963	1.00	165.64
2273 2274	Ň	VAL A	96	-6.044	33.966	6.222	1.00	165.64
40 2275	CA	VAL A	96	-6.778 -7.256	32.573	6.592	1.00	130.98
2276	CB	VAL. A	96 96	-8.370	32.683	7.632	1.00	130.98 130.98
2277	CG1	VAL A	96	-7.722	31.830	5.359	1.00 1.00	165.64
2278	CG2	VAL A VAL A	96	-5.864	34.458	7.335 7.475		165.64
2279	C	VAL A	96	-4.743	33.962	8.147		117.82
45 2280	N	VAL A	97	-6.339	35.404 35.949	9.204		117.82
2281 2282	CA CA	VAL A	97	-5.483	35. 545 37. 299	8.784	1.00	171.13
2283	СВ	VAL A	97	-4.908 -3.692	37.597	9.605		171.13
2284	CG1	VAL A	97	-3.652 -4.577	37.296	7.30		171.13 117.82
50 2285	CG2	VAL A	97 97	-6.078	36.149	10.58		117.82
2286	C	VAL A VAL A	97	-7.269	36.404	10.71 11.60		130.77
2287	0	MET A		-5.221	36.046	13.02	-	130.77
2288	N CA	MET A		-5.592	36,228 35,504	13.92		249.69
2289 55 2290	CB	MET A	98		33.992	13.78	5 1.00	249.69
2291	ČĠ	MET A			33.193	14.58		249.69
2292	Œ	MET A	98	- 400	33.351	16.32		249.69 130.77
2293	CE	MET A	98 39 /		37.712	13.30		130.77
2294	Ç	MET A		4 = 400	38.332	13.11		130.20
60 2295	0	GLU /			38.276	13.8 14.1		130.20
2296	N CA	GLU /		-6.679		15.1	T	216.65
2297	CB	GLU A	A 95	9 <i>-7.77</i> 3	39.989 41.423	15.1		216.65
2298 2299	cG	GLU	A 9	- 444		16.3	55 1.00	216.65
65 2300	CD	GLU	A 9		40.074	16.7	95 1.00	216.65
2301	OE.		-			16.8		216.65 130.20
2302	OE	gLU		19 -9.080 19 -5.34°	*	14.7		400.00
2303	Ç	GLU	••	9 -4.83	2 39.538	15.0	572 1.00 157 1.00	
2304		GLY	• -	00 -4.75		14.	15/ 1.00	
70 2305	, 14	42.	-	•				

	2306 2307 2308 2309 2310 2311	CA C O N CA CB	GLY A GLY A GLY A GLN A GLN A GLN A GLN A	100 100 100 101 101 101	-3.476 -2.232 -1.210 -2.305 -1.173 -1.385 -1.255	41.685 41.342 42.016 40.305 39.891 38.471 37.429	14.674 13.8 6 9 13.999 13.043 12.209 11.699 12.777 13.650	1.00 1.00 1.00 1.00 1.00 1.00 1.00	150.30 150.30 150.30 149.89 149.89 220.06 220.06
	2312	CD CG	GLN A	101 101	-0.056 -0.048	37.694 38.646	14.431 13.516	1.00 1.00	220.06 220.06
	2313 2314	OE1	GLN A GLN A	101	0.974	36.862 40.831	11.033	1.00 1.00	149.89 149.89
10	2315 2316	NE2 C	GLN A	101 101	-0.918 -1.663	41.773	10.795 10.277	1.00	131.84
	2317	0 N	GLN A PRO A	102	0.161 1.289	40.572 39.692	10.571	1.00 1.00	202.39 131.84
	2318 2319	CD	PRO A	102 102	0.440	41.436 41.376	9.131 9.067	1.00	202.39 202.39
15	2320	CA CB	PRO A	102 102	1.966 2.222	39.941	9.395 7.837	1.00 1.00	131.84
	2321 2322	CG C	PRO A	102	-0.216 -0.418	40.960 39.749	7.627	1.00 1.00	131.84 120.38
	2323 2324	0	PRO A	102 103	-0.531	41.915 41.589	6.960 5.695	1.00	120.38 119.50
20	2325	N GA	LEU A	103	-1.150 -2.620	41.909	5. 782 4.569		119.50
	2326 2327	CB	LEU A LEU A	103 103	-3.321	41.329 39.821	4.686	1.00	119.50 119.50
	2328 2329	CG CD1	LEU A	103 103		41.816	4.475 4.508		120.38
25	2330	CD2 C	LEU A	103	-0.542	42.345 43.582	4.53	7 1.00	120.38 130.73
	2331 2332	0	LEU A	100	-0.116	41.629 42.300	3.46 2.28	8 1.00	130.73 196.69
	2333	N CA	PHE /	10		42.002	2.14 3.35		196.69
30	2334) 2335	CB CG	PHE PHE	À 10	4 2.747	42.332 41.480	4.44	1.00	196.69 196.69
-	2336 2337	CD1		A 10	3.493	43,499	3.4° 5.5	1.00	196.69
	2338	CD2 CE1	PHE	19	3.495	41.787 43.815	4.5 5.6		196.69
3	2339 5 2340	CE2	PHE	Ä 1	04 4.238	42.960 41.868	1.0	04 1.00	0 130.73
_	2341 2342	CZ C	PHE	A 1	04 -0.236 04 -0.279	40.673	0.6 0.2	₂₅₈ 1.0	0 119.49
	2343	0 N	PHE	1	05 -0.774		-1.0	1.0	no 119.62
	2344 40 2345	CA	LEU LEU		05 -2.813	43.107	0.	049 1.0	00 119.62
	2346 2347	CB CG	LEU	Α ΄	105 -3.73! 105 -5.13	43.152		172 1.0 063 1.0	00 119.62
	2348	CD1 CD2		•	105 -3.73	8 41.002	-2	.137 1.0	00 119.49 00 119.49
	2349 45 2350	C	LEL	A J A	105 -0.57 105 0.09	44.104	_	291 1.	00 119.67
	2351	0 N	AR	3 A	106 -0.61		4		00 158.51
	2352 2353	CA	·	G A G A	106 1.5	10 42.10	, .	5.412 1	.00 158.51
	2354 50 2355		AR AR	G A	106 2.5 106 3.6	56 41.50	3 -		158.51
	2356	GE ST	. AF	IG A IG A	106 4.5		, 6 .	7.233	1.00 158.51 1.00 158.51
	2357 2356	CZ	Z AF	RG A RG A	106 5.1	180 39.60	r r 10	-8.280	1.00 158.51
	235	9 NI	H2 A	RG A		505 42.80	8		1 00 119.67
	236	1 6	A	rg a rg a	106 -1.	026 41.7		-6.455	1.00 120.58 1.00 120.58
	236 236	33 N	í	YS A	107 -1	189 43.9	04	-7.774 -8.666	1.00 120.58
	230	54 S	<u>~</u>	YS A	107 -0	.053 43.4 .836 44.2	99	-8.953 -8.168	1.00 140.98
	60 23 23	66	o 9	CYS A	107 -1	.645 45.3		-9.622	1.00 140.98 1.00 148.29
	23 23	168	sa (CYS A		069 42.	210	-9.083 -9.914	1.00 148.29
	23	369		HIS A HIS A	108	1.002 41.1 1.309 40.	222	-9.470	1.00 171.13 1.00 171.13
		370 371	CB	HIS A		2.556 ^{39.}	.660 .483	-10.068 -10.691	1.00 171.13
	2	372	CO2	HIS A	108 108	2.753 3.773 40	.308	-10.001 -10.548	1.00 171.13 1.00 171.13
	2	373 374	ND1 CE1	HIS A	108	4.702 39	.549	- 10,010	
	70 2	2375	~~·						

										171.13
					4.136	38.4		-10.975	1.00 1.00	148.29
	2376	1100	HIS A HIS A	108 108	0.759	41.6		-11.411 -11.896	1.00	148.29
	2377	Ŏ.	HIS A	108	-0.248	41.0 42.2		-12.136	1.00	189.63 189.63
	.2378 2379	N .	GLY A	109	1.701 1.593	42.2		-13.579	1.00 1.00	189.63
5	2380	CA	GLY A	109 109	2.109	41.0		-14.172 -13.469	1.00	189.63
3	2381	C	GLY A	109	2.735	40.	217 782	-15.454	1.00	151.88
	2382	0 N	TRP A	110	1.836 2.302		582	-16.136	1.00	151.88 208.61
	2383 2384	CA	TRP A	110 110	1.381	39.	246	-17.307 -18.184	1.00 1.00	208.61
10	2385	СВ	TRP A	110	1.896		.147	-18.170	1.00	208.61
••	2386	CG CD2	TRP A	110	1.495		.764 .100	-19.135	1.00	208.61 208.61
	2387 2388	CE2	TRP A	110 110	2.277 0.556	36	.022	-17.434	1.00 1.00	208.61
	2389	CE3	TRP A	110	2.863	38	3.255	-19.134 -19.708	1.00	208.61
15	2390	CD1 NE1	TRP A	110	3.103		7.034 4.723	-19.387	1.00	208.61 208.61
	2391 2392	CZ2	TRP A	110	2.147 0.429	34	4.653	-17.688	1.00 1.00	208.61
	2393	CZ3	TRP A	110 110	1.218		4.024	-18.658 -16.615	1.00	151.88
	2394	CH2	TRP A	110	3.747		9.773 0.909	-16.869	1.00	151.88 149.24
20	2395	C O	TRP A	110	4.182 4.490		8.666	-16.714	1.00 1.00	149.24
	2396 2397	Ň	ARG A	111	5.892		8.712	-17.125 -18.619	1.00	249.69
	2398	CA	ARG A ARG A	111	6.013	1 3	39.012	-19.494	1.00	249.69
	2399	CB CG	ARG A	111	6.011		37.777 38.106	-20.902	1.00	249.69 249.69
25	2400 2401	CD	ARG A	111 111	6,475 7,340	,	37.059	-21.427	1.00 1.00	249.69
	2402	NE	ARG A	111	- 400	o :	36.693	-20.868 -19.757	1.00	249.69
	2403	CZ	ARG A	111	8.916	9	37.285 3 5.72 1	-21.411	1.00	249.69 149.24
20	2404	NH1 NH2	ARG A	111			39.777	-16.336	1.00 1.00	149.24
30) 2405 2406	C	ARG A	11°			40.391	-16.825 -15.107	1.00	174.92
	2407	0	ARG A ASN A	11:	2 6.21		39.988 40.958	-14.231	1.00	174.92 206.21
	2408	N CA	ASN A	11			40.434	-13.735		206.21
3:	2409 5 2410	CB	ASN A	11 11			41.184	-12.514 -12.171		206.21
٠,	2411	CG	ASN A ASN A	11	2 8.2		42.256 40.620	-11.858	1.00	206.21 174.92
	2412	OD1 ND2	ASN A	. 11	12 9.7 12 7.0		42.293	-14.93	7 1.00	174.92
	2413 2414	С	ASN A	•	12 7.0 12 7.9		43.001	-14.64 -15.86		198.50
4	O 2415	0	ASN A	•	13 6.1	29	42.643 43.932	-16.54	7 1.00	198.50
	2416	N CA	TRP /	1		233 232	43.932	-17.67		235.99 235.99
	2417 2418	CB	TRP			ಬಾ 869	43.414	-18.92 -19.89		235.99
	2419	CG			113 4.	825	42.775	-20.96	55 1.00	
	45 2420	CD2 CE2	TRP	Ä	113 5.	653 455	42.372 42.498	-19.9	49 1.00	22E 00
	2421 2422	CE3	TRP	Α ΄		.927	43.381	-19. 4 -20.6	40 1.00 65 1.00	235.99
	2423	CD1	TRP TRP			.931	42.753	-20.0 -22.0	•	235.99
	2424	NE1 CZ2			113 5	.150	41.705 41.837	-21.0	67 1.0	
	50 2425 2426	CZ3	TRP	A		.952 3.801	41.452	-22.1		198.50
	2427	CH2	TRP TRP			.948	45.050	-15.5 -14.3		O 198.50
	2428	CO	TRP		113	5.891	44.821 46.262	-16.	069 1.0	
	55 2430		ASP	Α	• • •	5.765 5.476	47.388	-15.		040.60
	2431	CA	ASP ASP	A		6.471	48.542	-15. -14	692 1.0	00 249.69
	2432		400		114	7.802	48.353 48.237		446 1.	00 249.69
	2433 2434	,	ASF	• A		7.791 8.863	48.329			00 249.65
	60 243	5 00	₁₂ ASF	? A	114 114	4.037	47.881	46		no 220.71
	243	6 C		? A ? A	114	3.569	48.065 48.072	-14	.242	.00 122.27
	243		VA	LA	115	3.337 1.960	48.556	-14	7.200	.00 122.27 .00 142.42
	243 243	ig C	`	LA	115 115	1.032	47.648	-15		00 142.42
	65 244	ω Q		L A L A	115	-0.418	47.957 46.195		3,716 ¹	.00 142.42
	244	*' ∼	Go VA	L A	115	1.328 1.889	49.97	á -1	3.705	400 07
	24 24	43 C	V/	T V	115 115	2.566	50.31	1 -]		1.00 122.27 1.00 125.74
	24	44 C	-	ALA (RA	116	1.061	50.80	0 •1	7.000	
	70 24	45 N								

	2446 2447	CA CB CG	TYR A TYR A TYR A	116 116 116	0.885 1.328 2.797	52.181 53.115 53.014 52.218	-13.923 -15.058 -15.357 -16.397	1.00 1.00 1.00 1.00	125.74 233.81 233.81 233.81 233.81
	2448 2449	CD1	TYR A	116 116	3 <i>.2</i> 72 4.644	52.092	-16.639 -14.568	1.00 1.00	233.81
. 5	2450	CE1	TYR A	116	3.720	52 683 53.566	-14.796	1.00	233.81
-	2451	CD2 CE2	TYR A	116	5.089 5.551	52.773	-15.832	1.00 1.00	233.81 233.81
	2452 2453	CZ	TYR A	116 116	6.914	52.664	-16.054 -13.539	1.00	125.74
	2454	OH	TYR A TYR A	116	-0.578	52.470 51.626	-13.747	1.00	125.74
10	2455	C O	TYR A	116	-1.451	53.665	-12.992	1.00 1.00	145.27 145.27
	2456 2457	Ň	LYS A	117 117	-0. 83 3 -2.176	54.095	-12.584 -13.801	1.00	191.01
	2458	CA	LYS A LYS A	117	-3.020	54.515	-14.267	1.00	191.01
	2459	CB CG	LYS A	117	-2.807	55.955 56.437	-15.140		· 191.01 191.01
15	2460 2461	CD	LYS A	117 117	-3.969 -5.304	56.363	-14.377 -15.161		191.01
	2462	CE	LYS A LYS A	117	-6.504	ge 911	-11.814	1.00	145.27
	2463	NZ C	LYS A	117	-2.913	53.014 52.653	-12.141	1 1.00	145.27 149.03
20	2464	Ö	LYS A	117	-4.053 -2.269	52.518	-10.767		149.03
20	2465 2466	N	VAL A VAL A	118 118	-2.858	51.469	-9.959 -9.35		99.24
	2467	CA	VAL A VAL A	118	-1.761	50.802 49.921	-8.08	1 1.00	99.24 99.24
	2468	CB CG1	VAL A	118	-2.233 -1.364	49.558	-10.37		149.03
25	2469 2470	CG2	VAL A	118 118	-3.816	51.912	-8.85 -8.17		149.03
25	2471	Ç	VAL A	118	-3.601	52.931 51.115	-8.70	6 1.00	111.23
	2472	O N	ILE A	119	-4.878	51.115 51.325	-7.7	14 1.00	111.26 110.34
	2473 2474	CA	ILE A	119 119		51.950	-8.39 -7.2		110,34
30		CB	ILE A	119	- 400	52.293	-7.2 -9.1	08 1.00	110.34
50	2476	CG2 CG1	ILE A	119	9 -6.752	53.187 53.537	-10.1	66 1.00	110.34 111.26
	2477 2478	CD1	ILE A	- 44		49.972	-7.1 -7.9	_	111.26
	2479	Ç	ILE A		9 -6.641	49.054 49.843	-7.5 -5.8	848 1.00	126.83
3:	5 2480	0 N	TYR A	12	0 -6.378	40.003		266 1.00	400.40
	2481 2482	GA CA	TYR A	12	20 -6. 82 9 20 -6.039	48.270		015 1.00 280 1.00	126.10
	2483	CB	TYR /	•	20 -4.615	47.904		399 1.0	0 126.10
	2484	CG CD1		À 1	20 -3.636		-4.	.657 1.0	
4	O 2485 2486	CE1	TYR		20 -2.315 20 -4.24	40 560		.427 1.0 .687 1.0	
	2487	CD2			20 -2.93	0 46.213		.802 1.0	126.10
	2488	CE2	TYR TYR	1	20 -1.96		-5	.067 1.0	
	2489	CZ OH	TYR	A 1	20 -0.66	40.040		1.889 1.0 4.606 1.0	400.00
•	45 2490 2491	C	TYR TYR		120 -8.26 120 -8.67	2 49.956	,		00 10 0 .78
	2492	0	TYR	, ,	121 - 9 .0		,	4.516 1.	00 106.78 00 155.39
	2493	N CA	TYR	Α	121 -10.4	47 72	•	J., J.	00 155.39 00 155.39
	2494 50 2495	СВ	TYR	A	121 -11.4 121 -11.3	₆₂ 48.83	,		00 155.39
	2496	CG	TYR TYR		121 -10.1	81 49.12	<u> </u>	-8.499 1	.00 155.39 .00 155.39
	2497		TYR	A	121 -10.1 121 -12.5	70	2		00 155.39
	2498 2499	CD	2 TYP		121 -12. 121 -12.	196 5U.4C	• •		100 100.39
	55 2500	CE.		A	121 -11.	309 50.75		-9.903	1.00 155.39 1.00 106.78
	2501		TY	A F	121 -11. 121 -10.	40 04		-00-	100 106.78
	2500 2500	_	TY	R A	121 -10. 121 -10.	RAA 45.6			1.00 141.82
	250	4 0	17	R A S A	122 -11	.618 47.2		1.440	1.00
	60 250		LY لم	SA		,100	174	-0.000	040.21
	250 250	~	B LY	SA	122 -11 122 -11	983 45.7	716	0.997 2.367	1.00 249.31
	250	% C	G LY	'S A 'S A	122 -11	.631 40-		3.451	1.00 249.31
	250	₀₉ C		'S A	122 -13		380 00 5	4.773	1.00
	65 25° 25		iz Ľ	(S A		3.631 46.	511	-1.375 -1.042	1.00 141.82
		12	;	ys a Ys a	122 -1	4.136 47.	.587 .433	-1.703	1.00 127.31
	25	13	ú A	SP A	123 -1	-7.0	.435 .436	-1.701	1.00 127.31
			CA A	SP A	123 -1	5.801 45			
	,,,	-							

				_				-0.276	1.00	199.26
			ASP A	123	-16.344		.574	0.531	1.00	199.26
	16		ASP A	123	-16.186		.302 3.223	0.031	1.00	199.26
	517		ASP A		-16.571		1.223 1.378	1.668	1.00	199.26
	18	OD1 OD2	ASP A	123	-15.685	'	3.531	-2.584	1.00	127.31
	519	C	ASP A	123	-16.395	, a.	7.311	-2.132	1.00	127.31
	520	ŏ	ASP A	123	-17.238		8.579	-3.842	1.00	152.83
	521	N	GLY A	124	-15.95		7.561	-4.788	1.00	152.83 152.83
	522	CA	GLY A	124	-18.46	,	9.007	-4.590	1.00	152.83
	523	C C	GLY A	124	-16.06 -16.39	٠ .	9.847	-5.425	1.00	121.95
	524 525	ŏ	GLY A	124	-15.35	"	9.297	-3.502	1.00 1.00	121.95
	2526	N	GLU A	125 125	-14.91		60.668	-3.185	1.00	249.20
	2527	CA	GLU A	125	-15.03	17 5	0.926	-1.673	1.00	249.20
	2528	CB	GLU A	125	-16.46	i4 :	51.006	-1.143 -1.519	1.00	249.20
	2529	CG	GLU A	125	-17.15	54	52.304	-1.081	1.00	249.20
	2530	CD	GLU A	125	-16.6		53.373	-2.250	1.00	249.20
	2531	OE1	GLU A	125	-18.1	68	52.253	-3.612	1.00	121.95
	2532	OE2	GLU A	125	-13.4	, ,	50.956	-3.548	1.00	121.95
	2533	C	GLU A	125	-12.6		50.071 52.185	-4.059	1.00	117.59
	2534	O N	ALA A	126	-13.2		52.103	-4.444	1.00	117.59
20	2535	CA	ALA A	126	-11.8		53.935	-5.116	1.00	242.07
	2536	CB	ALA A	126	-11.9		52.638	-3.12 9	1.00	117.59 117.59
	2537	Č	ALA A	126		102	53.123	-2.132	1.00	119.50
	2538 2539	ŏ	ALA A	126		B62	52.176	-3.112	1.00	119.50
25	2540	Ň	LEU A	127	_	140	52.177	-1.857	1,00 1,00	117.16
23	2541	CA	LEU A	127 127	_	845	50.751	-1.411	1.00	117.16
	2542	CB	LEU A	127	_	750	50.671	0.099 0.705	1.00	117.16
	2543	CG	LEU A	12		045	51.245	0.705	1.00	. 117.16
	2544	CD1	LEU A	12		.534	49.234	-1.813	1.00	119.50
30	2545	CD2	LEU A	12		.859	52.960	-1,030	1.00	119.50
	2546	C	LEU A	12	7 -7	.738	53.890	-2.616	1.00	140.05
	2547	0	LYS A	12		.880	52.566 53.269	-2.661	1.00	140.05
	2548	N CA	LYS A	12		.603	52.411	-2.036	1.00	182.59 182.59
	2549	CB	LYS A	12		.503	52.060	-0.576	1.00	182.59
35	2550	cG	LYS A			1.725 1.526	53.260	0.337		182.59
	2551	ČD	LYS A			4.526 4.657	52.855	1.80		182.59
	2552 2553	CE	LYS A			4.240	53.938	2.74		140.05
	2554	NZ	LYS A			5.293	53.534	-4.12		140.05
40	2555	С	LYS A	•		5.875	52.899	-5.01 -4.39		141.11
40	2556	0	LYS A	•		4.386	54.467	-4.38 -5.77		141.11
	2557	N	TYR	•	29	4.021	54.780	-6.34		146.88
	2558	CA			129	-4.977	55.812	-7.57		146.88
	2559	CB			129	-4.437	56.491 55.909	-8.8		146.88
45		CG CD1		À	129	-4.560	56.518	-9.9	57 1.00	146.88 146.88
	2561	CE1		Α	129	-4.010	57.705	-7.4	74 1.00	440.00
	2562	CD2		A	129	-3.749	58.313	-8.5	93 1.00	
	2563	CE2		Α	129	-3.191	57.717	-9.8		
50	2564) 2565	CZ		A	129	-3.327 -2.781	58.324	-10.9		
)(2566	OН		Ą	129	-2.588	55.294	-5.9		
	2567	C	TYR	Ą	129 129	-2.098	56.070	-5.1		407 60
	2568	0	TYR	A	130	-1.919	54.861		014 1.00 282 1.00	137.60
	2569	N	TRP	Ä	130	-0.545	55.292	-/ -8	821 1.0	D 197.40
5	5 2570	CA	TRP TRP		130	0.487	54.377		190 1.0	0 197.40
	2571	CB	TRP	2	130	0.244	54.027		060 1.0	0 197.40
	2572		700		130	0.940	54.526		911 1.0	0 197.40
	2573				130	0.426	53.878 55.458		.892 1.0	0 197.40
	2574		TRP	Α	130	1.974	55,458 53,124		.702 1.0	0 197.40
•	50 2575		~ ~~~	A	130	-0.661	53.124	-3	.335 1.0	
	2576		TRF	• A	130	-0.561	54,128		.624 1.0	407.40
	2577	~~	TRF	2 A	130	0.893	55.713	2	2.598 1.0	
	2578 2579	,	- TRI	> A	130	2.452 1.906	55:055	-1		
	65 258		42 TRI	PA	130	-0.262	55.287	, -1		00 137.60 00 137.60
	258	~	TR	PA	130 130	-1.055	54.764			00 159.17
	258 258	` ~	TR	PA	131	0.879	55.86	, ,	0.100	.00 159.17
	258	ß N		RA	131	1.313	55.92	•	0.554 1 0.798 1	.00 169.09
	258	₁₄ C	·` —	RA	131	2,164		5 •1	V.730 '	
	70 258		в 17	n ^						
	<i>-</i>									

	2586 2587	CG CD1 CE1:	TYR A TYR A TYR A	131 131 131	2.407 1.394 1.603	57. 58.	426 ,927 ,144 ,150	-12.241 -13.051 -14.415 -12.821	1.00 1.00 1.00 1.00	169.09 169.09 169.09
	2588 2589 2590 2591 2592	CD2 CE2 CZ OH C	TYR A TYR A TYR A TYR A TYR A	131 131 131 131	3.642 3.863 2.842 3.073 2.152 1.619	57 57 58 54	.363 7.858 3.051 4.655 3.613	-14.183 -14.974 -16.318 -10.756 -11.140	1.00 1.00 1.00 1.00 1.00 1.00	169.09 169.09 169.09 159.17 159.17 172.97
10	2593 2594 2595 2596 2597 2598	O N CA CB CG	TYR A GLU A GLU A GLU A GLU A	131 132 132 132 132 132	3.464 4.328 5.777 6.593 7.78	55 55 55 55 55 55	4.754 3.577 3.933 4.598 3.750	-10.524 -10.594 -10.237 -11.341 -11.767 -11.058	1.00 1.00 1.00 1.00 1.00	172.97 249.69 249.69 249.69 249.69
15	2599 2600 2601 2602 2603	OE1 OE2 C	GLU A GLU A GLU A GLU A ASN A	132 132 132 132 133	8.09 8.41 3.67 3.53 3.28	1 5 7 5 11 5	52.767 54.063 52.838 53.413 51.580 50.925	-12.804 -9.436 -8.343 -9.628 -8.545	1.00 1.00 1.00 1.00 1.00	249.69 172.97 172.97 204.08 204.08 217.94
20	2604 2605 2606 2607 2608	N CA CB CG OD1 ND2	ASN A ASN A ASN A ASN A	133 133 133 133 133	2.55 1.83 2.70 3.80 2.1	39 05 62 14	49.637 48.389 48.418 47.262 50.722	-9.065 -9.085 -9.493 -8.676 -7.190	1.00 1.00 1.00 1.00 1.00	217.94 217.94 217.94 217.94 204.08 204.08
25	2609 2610 2611 2612 2613 2614	C O N CA CB	ASN A ASN A HIS A HIS A	133 133 134 134 134	2.4	22	51.214 50.050 49.818 50.910 50.881	-6.922 -6.314 -4.979 -4.067 -2.679	1.00 1.00 1.00 1.00 1.00 1.00	188.50 188.50 249.69 249.69 249.69
30		CG CD2 ND1 CE1 NE2	HIS A HIS A HIS A HIS A HIS A HIS A	134 134 134 134 134	4.4.4.4.4.3.	405 338 557 399 485	50.671 51.055 50.953 50.720 48.456	-1.481 -2.429 -1.120 -0.530 -4.542 -5.374	1.00 1.00 1.00 1.00	249.69 249.69 249.69 188.50 188.50
35	2620 2621 2622 2623 2624	C O N CA CB	HIS A ASN A ASN A ASN A ASN A	13 13 13	4 2 5 2 5 2 5 3 35 3	.068 .518 .076 .274 3.803	47.636 48.217 46.946 45.986 45.530	-3.234 -2.670 -2.547 -3.900 -4.770	1.00 1.00 1.00 1.00 1.00 1.00	249.69
4	2626 2627 2628 2629	CG OD1 ND2 C O N	ASN A ASN A ASN A	13 14 15 14 16 17	35 35 35 36	3.010 5.128 1.431 2.081 0.151	45.158 45.534 47.190 47.042 47.572 47.846	-4.08 -1.30 -0.27 -1.31 -0.11	6 1.00 1 1.00 1 1.00 3 1.00 15 1.00	122.11 122.11 110.87 110.87
	2630 2631 2632 2633 2634	CA CB CG2 CG1 CD1	ILE ILE ILE	A 1 A 1 A	136 136 136 136	0.653 -2.147 -2.474 -2.973 -4.463	47.756 46.406 47.969 47.811 46.912	-0.45 -1.05 0.8 0.5 1.0	55 1.0 01 1.0 53 1.0 75 1.0	0 153.19 0 153.19 0 153.19 0 110.87
;	50 2635 2636 3537 2638 2639 55 2640	C O N CA CB	SER SER SER	A A A	136 137 137 137	-0.350 -0.773 0.351 0.763 2.242 2.597	45.732 47.475 46.734 46.951 46.432	3.4 4.7)61 1.0 254 1.0 488 1.0 746 1.0	00 139.22 00 139.22
	2841 2642 2843 2844 60 2845	O N CA		AAAA	137 137 137 138 138 138	0.032 -0.378 -0.080 -0.760 -2.136	47.027 48.149 45.991 46.072 45.423	4. 5. 6. 6.	823 1. 374 1. 659 1. 577 1	00 139.22 .00 158.60 .00 158.60 .00 139.81 .00 139.81
	2646 2647 264 264 65 265 265	6 CB 7 CG 8 CG 9 CC	12 ILE 11 ILE 11 ILE 1LE 1LE	. A	138 138 138 138 138	-2.695 -3.058 -4.349 0.014 0.321 0.309	45.183 46.314 45.652 45.396 44.200 46.174	5 5 7 3	.766 1 .392 1 .780 1 .716 3	.00 139.81 .00 139.81 .00 158.60 1.00 158.60 1.00 172.47 1.00 172.47
	265 265 265 266 70 26	N 33 C 54 C	TH' A TH B TH	R A R A R A	139 139 139 139	1.053 1.698 0.689	45.69 46.87 47.85	5 7	0.697	1.00 249.69 1.00 249.69

2677 C THR A 142 -8.849 43.153 10.277 1.00 16 2678 O THR A 142 -8.244 43.310 12.037 1.00 16) 7 7
2659 N ASN A 140 -1.573 45.233 12.882 1.00 189.0 5 2660 CA ASN A 140 -1.738 46.209 13.830 1.00 189.0 2661 CB ASN A 140 -2.767 45.750 14.835 1.00 189.0 2662 CG ASN A 140 -3.887 45.750 14.466 1.00 189.0 2663 OD1 ASN A 140 -2.877 45.403 11.466 1.00 189.0 2664 ND2 ASN A 140 -2.877 45.113 11.879 1.00 189.0 2666 C ASN A 140 -3.367 46.110 11.335 1.00 189.0 2666 O ASN A 140 -3.367 46.110 11.335 1.00 189.0 2667 N ALA A 141 -3.437 43.904 11.818 1.00 161. 2668 CA ALA A 141 -4.669 43.674 11.062 1.00 161. 2669 CB ALA A 141 -4.569 42.364 10.287 1.00 147. 2668 CB ALA A 141 -5.962 43.694 11.874 1.00 161. 2671 O ALA A 141 -5.962 43.694 11.874 1.00 161. 2671 O ALA A 141 -6.105 42.992 12.888 1.00 161. 2672 N THR A 142 -6.902 44.510 11.402 1.00 148. 2673 CA THR A 142 -8.208 44.652 12.032 1.00 148. 2674 CB THR A 142 -8.208 46.049 11.793 1.00 197. 2675 OG1 THR A 142 -8.208 46.049 11.793 1.00 197. 2676 CG2 THR A 142 -8.208 46.049 11.793 1.00 197. 2677 CG THR A 142 -8.208 43.636 11.376 1.00 197. 2677 C THR A 142 -8.208 43.636 11.376 1.00 197. 2677 C THR A 142 -9.126 43.636 11.376 1.00 144. 26777 C THR A 142 -9.126 43.636 11.376 1.00 144. 26777 C THR A 142 -9.126 43.636 11.376 1.00 166. 2678 O THR A 142 -8.849 43.153 12.037 1.00 166.	
5 2660 CA ASN A 140 -1.738 45.750 14.835 1.00 189.0 2661 CB ASN A 140 -2.767 45.403 14.466 1.00 189.0 2662 CG ASN A 140 -3.887 45.403 14.466 1.00 189.0 2663 OD1 ASN A 140 -2.877 45.113 11.879 1.00 189.0 2664 ND2 ASN A 140 -2.877 45.113 11.879 1.00 189.0 10 2665 C ASN A 140 -2.877 45.113 11.879 1.00 189.0 2666 O ASN A 140 -3.357 46.110 11.335 1.00 161. 2667 N ALA A 141 -3.437 43.674 11.062 1.00 161. 2667 N ALA A 141 -4.569 42.364 11.874 1.00 161.	0
2661 CG ASN A 140 -2.767 45.403 14.466 1.00 189.0 2662 2663 OD1 ASN A 140 -3.887 45.764 16.111 1.00 189.0 2664 ND2 ASN A 140 -2.877 45.113 11.879 1.00 189.0 10 2665 C ASN A 140 -2.877 46.110 11.335 1.00 189.0 2666 O ASN A 140 -3.367 46.110 11.335 1.00 161. 2666 N ALA A 141 -3.437 43.904 11.818 1.00 161. 2667 CA ALA A 141 -4.669 42.364 10.287 1.00 161. 2668 CB ALA A 141 -4.569 42.364 10.287 1.00 161. 2669 CB ALA A 141 -5.962 43.694 11.874 1.00 161. 2669 CB ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 O ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 O ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 O THR A 142 -6.902 44.510 11.402 1.00 148. 2671 CA THR A 142 -8.208 44.652 12.032 1.00 148. 2672 CA THR A 142 -8.208 46.049 11.793 1.00 197. 2673 CB THR A 142 -8.208 46.049 11.793 1.00 197. 2675 CG2 THR A 142 -7.820 47.046 12.140 1.00 197. 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1	
2863 OD1 ASN A 140 -2.398 45.764 10.111 1.00 189.1 2664 ND2 ASN A 140 -2.877 45.113 11.879 1.00 189.1 10 2665 C ASN A 140 -3.367 46.110 11.335 1.00 189.1 2666 O ASN A 140 -3.367 43.904 11.818 1.00 161. 2667 N ALA A 141 -3.437 43.904 11.818 1.00 161. 2667 N ALA A 141 -4.669 42.364 10.287 1.00 147. 2668 CA ALA A 141 -4.569 42.364 10.287 1.00 147. 2669 CB ALA A 141 -5.962 43.694 11.874 1.00 161. 2669 CB ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 O ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 O THR A 142 -6.902 44.510 11.402 1.00 148. 2672 N THR A 142 -8.208 46.649 11.793 1.00 197. 2673 CA THR A 142 -8.208 46.049 11.793 1.00 197. 2673 CB THR A 142 -8.208 46.049 11.793 1.00 197. 2675 OG1 THR A 142 -7.820 47.046 12.140 1.00 197. 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144. 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -8.849 43.153 10.277 1.00 164. 2677 C THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165. 2678 O THR A 142 -8.849 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 1.00 165. 2678 O THR A 143 -10.224 43.310 12.037 11.456 1.00	
2664 ND2 ASN A 140 -2.877 45.113 1.335 1.00 188.1 10 2665 C ASN A 140 -3.367 46.110 11.335 1.00 161. 2666 O ASN A 140 -3.437 43.904 11.818 1.00 161. 2667 N ALA A 141 -3.437 43.904 11.062 1.00 161. 2668 CA ALA A 141 -4.669 43.674 11.062 1.00 147. 2668 CB ALA A 141 -4.569 42.364 10.287 1.00 161. 2669 CB ALA A 141 -5.962 43.694 11.874 1.00 161. 2670 C ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 O ALA A 141 -6.105 42.992 12.888 1.00 161. 2672 N THR A 142 -6.902 44.510 11.402 1.00 148. 2673 CA THR A 142 -8.208 44.652 12.032 1.00 197. 2673 CA THR A 142 -8.208 44.652 12.032 1.00 197. 2674 CB THR A 142 -8.208 46.049 11.793 1.00 197. 2675 OG1 THR A 142 -7.820 47.046 12.140 1.00 197. 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -8.849 43.153 10.277 1.00 164. 2678 O THR A 142 -8.849 43.153 12.037 1.00 165.	
10 2665	
2686 2667 N ALA A 141 -4.669 43.674 10.087 1.00 147. 2668 CA ALA A 141 -4.569 42.364 10.287 1.00 147. 2669 CB ALA A 141 -4.569 42.364 11.874 1.00 161. 2669 CB ALA A 141 -5.962 43.694 11.874 1.00 161. 2670 C ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 O ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 C A THR A 142 -6.902 44.510 11.402 1.00 148. 2672 CA THR A 142 -8.208 44.652 12.032 1.00 197. 2673 CB THR A 142 -8.208 46.049 11.793 1.00 197. 2674 CB THR A 142 -7.820 47.046 12.140 1.00 197. 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -8.849 43.153 10.277 1.00 166 2678 O THR A 143 -10.224 43.310 12.037 11.00 167.	
2668 CA ALA A 141 -4.569 42.364 10.287 1.00 161. 2668 CB ALA A 141 -5.962 43.694 11.874 1.00 161. 2669 C ALA A 141 -5.962 43.694 11.874 1.00 161. 2670 C ALA A 141 -6.105 42.992 12.888 1.00 161. 2671 O ALA A 141 -6.105 42.992 12.888 1.00 161. 2672 N THR A 142 -6.902 44.510 11.402 1.00 148. 2673 CA THR A 142 -8.208 44.652 12.032 1.00 197. 2673 CA THR A 142 -8.792 46.049 11.793 1.00 197. 2674 CB THR A 142 -7.820 47.046 12.140 1.00 197. 2675 CG2 THR A 142 -7.820 47.046 12.140 1.00 197. 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -8.849 43.153 12.037 1.00 167. 2678 O THR A 143 -10.224 43.310 12.037 1.00 167.	
2669 CB ALA A 141 -5.962 42.992 12.888 1.00 161 2677 C THR A 142 -9.126 43.636 12.037 1.00 148 2677 C THR A 142 -9.126 43.636 12.037 1.00 148 2677 C THR A 142 -9.126 43.636 12.037 1.00 149 2677 C THR A 142 -9.126 43.636 11.376 1.00 147 2677 C THR A 142 -9.126 43.636 11.376 1.00 144 2677 C THR A 142 -9.126 43.636 11.376 1.00 144 2677 C THR A 142 -9.126 43.636 12.037 1.00 167 2678 O THR A 142 -9.126 43.636 12.037 1.00 167 2678 O THR A 142 -9.126 43.636 12.037 1.00 167 2678 O THR A 142 -9.126 43.636 12.037 1.00 167 2678 O THR A 142 -9.126 43.636 12.037 1.00 167 2678 O THR A 142 -9.126 43.636 12.037 1.00 167 2678 O THR A 142 -9.126 43.636 12.037 1.00 167 2678 O THR A 142 -9.126 43.636 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126 43.310 12.037 1.00 167 2678 O THR A 142 -9.126	
15 2670	
2677 N THR A 142 -8.508 44.652 12.032 1.00 197 2673 CA THR A 142 -8.792 46.049 11.793 1.00 197 2674 CB THR A 142 -7.820 47.046 12.140 1.00 197 2675 OG1 THR A 142 -7.820 47.046 12.636 1.00 197 20 2675 CG2 THR A 142 -10.036 46.245 12.636 1.00 197 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144 2677 C THR A 142 -8.849 43.153 10.277 1.00 167 2678 O THR A 143 -10.224 43.310 12.037 1.00 167	
2673 CA THR A 142 -8.792 46.049 12.140 1.00 197 2674 CB THR A 142 -7.820 47.046 12.140 1.00 197 2675 OG1 THR A 142 -7.820 47.046 12.636 1.00 197 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144 2677 C THR A 142 -9.126 43.636 11.376 1.00 144 2677 C THR A 142 -8.849 43.153 10.277 1.00 167 2678 O THR A 143 -10.224 43.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 11.456 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 11.456 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 1.00 167 2678 O THR A 143 -10.224 13.310 12.037 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 12.03 1	
2674 CB THR A 142 -7.820 47.040 12.636 1.00 197. 20 2675 OG1 THR A 142 -10.036 46.245 12.636 1.00 144. 2676 CG2 THR A 142 -9.126 43.636 11.376 1.00 144. 2677 C THR A 142 -8.849 43.153 10.277 1.00 167. 2678 O THR A 142 -8.849 43.310 12.037 1.00 167.	
20 2675 CG2 THR A 142 -10.050 43.636 11.376 1.00 144 2677 C THR A 142 -8.849 43.153 10.277 1.00 164 2678 O THR A 142 -8.849 43.310 12.037 1.00 167 2678 O THR A 143 -10.224 43.310 12.037 1.00 167 167 167 167 167 167 167 167 167 167	
2677 C THR A 142 -8.849 43.153 10.277 1.00 16 2678 O THR A 143 -10.224 43.310 12.037 1.00 16	3.72
2678 O IAI A 143 -10.224 43.310 11.456 1.00 16	7.20
2679 VAL A 145 -11.143 41.824 12.479 1.00 13	9.08 9.08
25 2680 CB VAL A 143 -13.146 42.910 12.826 1.00 13	9.08
2682 CG1 VALA 143 -12.838 40.590 10.334 1.00 16	7.20
2683 CG2 VAL A 143 -11.930 43.001 9.446 1.00 16	7.20 3.27
2684 VAL A 143 -12-432 10.372 1.00 1	3.27
30 2686 N GLU A 144 -12.785 45.043 9.742 1.00 2	19.50
2687 CA GILLA 144 -13.048 40.404 11.002 1.00 2	49.50 49.50
2688 CG GLU A 144 -13.660 47.202 12.141 1.00	49.50
2689 CD GLU A 144 -12.590 48.352 12.003 1.00 2	49.50
2691 OE1 GLU A 144 -12.888 46.511 8.019 1.00	93.27 93.27
2692 GLU A 144 -12,022 45,370 6,981 1,00	79.52
2693 O GLU A 144 - 10.755 44.606 8.069 1.00	79.52
40 2695 N ASP A 145 -9.931 44.524 7.228 1.00	162.18
2696 CA ASP A 145 -8.449 45 691 7.667 1.00	162.18 162.18
2697 CG ASP A 145 7.003 46.662 6.883 1.00	162.18
2899 OD1 ASP A 145 -7.286 45.750 6.766 1.00	179.52
45 2700 OD2 ASP A 145 -10.357 43.348 4.819 1.00	179.52 145.41
2701 O ASP A 145 -10.003 42.421 6.592 1.00	145.41
2702 N SER A 146 -11.10 41 223 5.886 1.00	152.87
2704 CA SER A 146 -12.318 40.267 7.907 1.00	152.87
50 2705 CB SER A 146 -11.477 39.510 4.782 1.00	145.41 145.41
2707 C SER A 146 -12.518 42.349 5.037 1.00	168.10
2708 O SER A 147 -12.323 41.140 3.457 1.00	168.10
2709 N GIV A 147 -13.215 41.47 1.149 1.00	168.10 168.10
55 2710 GLY A 147 -12.194 39.907 1.129 1.00	117.05
GLY A 17 42 206 41,428	117.05
2713 N THR A 148 -12.961 40.922 -2.014 1.00	146.29 146.29
2714 CR THR A 148 -14.209 41.446 -2.867 1.00	146.29
60 2/15 OG1 THR A 148 -15-327 40.059 -1.012 1.00	117.05
2717 CG2 THR A 148 -12.235 42.004 -2.502 1.00	117.05
2718 C THR A 148 -12.833 43.019 -2.386 1.00	131.53 131.53
2719 N TYR A 149 10.136 42.735 3.128 1.00	104.84
05 2720 CA TYR A 149 -8.772 42.906 -2.453 1.00	104.84
2722 CB TYR A 149 -8.803 43.338 0.010 1.00	104.84 104.84
2723 CD1 TYR A 149 9.127 42.823 1.361 1.00	(04.0
70 2725 CE1 TYR A 149 -9.127 42.823	

						_		-0.639	1.00	104.8	
				149	-8.477	44.6	43	0.700	1.00	104.8	
	2726	CD2	TYR A	149	-8.467	45.0 44.1	92 23	1.696	1.00	104.8	
	2727	CE2	TYR A	149	-8.792	44.5	:35	3.019	1.00	104.8 131.5	-
	2728	CZ. OH	TYR A	149	-8.778	42.		-4.589	1.00 1.00	131.	
_	2729	C	TYR A	149	-9.881 -10.064	41.		-4.989 5.063	1.00	105.	
5	2730	ŏ	TYR A	149 150	-9.454		380	-5.362 -6.784	1.00	105.	
	2731 2732	N	TYR A	150	-9.090		272	-7.660	1.00	139	
	2733	CA	TYR A	150	-10.319		023 .231	-7.964	1.00	139	
	2734	СВ	TYR A	150	-11.173		.210	-8.856	1.00	139 139	
10	2735	CG	TYR A	150	-10.738		.306	9.205	1.00	139	
	2736	CD1 CE1	TYR A	150	-11.568 -12.456		.369	-7.413	1.00 1.00	139	
	2737	CD2	TYR A	150	-12.430	45	.456	-7.759 -8.660	1.00	139	9.51
	2738 2739	CE2	TYR A	150 150	-12.839		5.418	-9.041	1.00		9.51
15	2740	CZ	TYR A	150	-13.648		7.469	-7.146	1.00		5.68
13	2741	OH	TYR A	150	-8.429		4.587 5.604	-6.525	1.00		5.68 19.57
	2742	C	TYR A	150	-8.720		4.585	-8.128	1.00		9.57
	2743	O N	CYS A	151	-7.536 -6.868		5.830	-8.510	1.00 1.00		99.57
	2744	N CA	CYS A	151			6.133	-9.992	1.00		99.57
20	2745	Č	CYS A	151	074	. 4	15.244	-10.786 -8.136	1.00		48.54
	2746 2747	Ö	CYS A	151 151		٠ 4	45.773	-8.958	1.00		48.54
	2748	CB	CYS A		4.440	3 '	44.452	-10.359	1.00		07.45
	2749	SG	CYS A	`	2 -6.782	-	47.396 47.838	-11.756	1.00		07.45 35.55
25		N	THR A	•	2 -6.857	,	48.753	-11.986	1.00		35.55
	2751	CA CB	THR /	15			50.045	-11.407	1.00 1.00		135.55
	2752	OG1	THR	15			48.160	-11.345	1.00	•	107.45
	2753 2754	CG2	THR				48.637	-12.118 -11.285			107.45
30		С	THR	•			49.358	-13.359	1.00		123.72
اد	2756	0	THR	Ā 1!	53 -5.15		48.518 49.241	-13.744	1.00		123.72 123.72
	2757	N	GLY		53 -3.97		49.248	-15.239			123.72
	2758	CA C	GLY	A 1	53 -3.74 53 -4.3		48.477	-15.96			129.98
_	2759	ŏ	GLY	A 1			50.113	-15.69 -17.10	•		129.98
3	5 2760 2761	Ň	LYS	· .	54 -2.8 54 -2.5		50.256	-17.10	•		212.29
	2762	CA	LYS		154 -2.4	190	51.740	-18.94	5 1.0		212.29
	2763	СВ	LYS LYS		154 -2.2	291	52.012 53.502	-19.22	25 1.0		212.29 212.29
	2764	cg	LYS	Ä	154 -2.		53.803	-20.69			212.29
4	40 2765	CD CE	LYS	Α		074 101	55.266	-20.9			129.98
	2766	117	ĹYS	•	,	179	49.591	-17.4 -16.9			129.98
	2767 2768	^	LYS			.130	49.969	-10.5			168.08
	2769		LÝS		155 -1	.242	48.579	-18.7	769 1.	00	168.08
	45 2770) N	JAV JAV		155 -0	.071	47.827 46.305	-18.7	759 1.	00	187.90 187.90
	277	t CA			,	.355	45.540	-19.		.00	187.90
	277				,,,,,).825).658	45.849	-17.		.00 .00	168.08
	277	· -	32 VA			D.193	48.277	-20. -21.		.00	168.08
	50 277	~	VA			0.717	48.244	-21. -20		.00	179.87
	277	76 O		- 4	156	1.429	48.672	-21	.834 `	.00	179.87
	277	77 N		RPA RPA	156	1.765	49.167 48.169		054	00.1	249.69 249.69
	27		· · · ·	A P	.00	1.399	46.890	-23		1.00 1.00	249.69
	27		TI O	RP A	156	2.200 3.591	46.752		,.000	1.00	249.69
	55 27	~	no T	RP A	156	3.900	45.367		3,302 3,714	1.00	249.69
		182 C	E2 T	RP A	156 156	4.606	47.657		2.774	1.00	249.69
		783	CE3	RP A	156	1.740	45.625 44.707		2.945	1.00	249.69 249.69
	27	784 S		RP A	156	2.754	44.871	-2	3.581	1.00	249.69
	60 2	785	NE1 CZ2	RP A	156	5.175	47.161		3.993	1.00 1.00	249.69
	2	,,,,	C73	TRP A	156	5.876 6.148	45.779	, -3	23.921	1.00	179.87
			OHO	TRP A	156 156	0.905	50.400	,	22.020 21.535	1.00	179.87
		789	Č.	TRP A	156	1.242	51.485	,	21.555 22.712	1.00	176.07
	65	2790	•	TRP A	157	-0.221	50.212	£	22.959	1.00	176.07 249.69
	05	2791	••	GLN A	157	-1.161	51.30 51.95	5 .	24.313	1.00	249.69
		2792	CA CB	GLN A	157	-0.864	52.85	. 1	24.311	1.00 1.00	249.69
		2793	CG	GLN A	157	0.381 0.232	- 4 07	' 8	-23.412	1.00	
		2794 2795	CD	GLN A	157	J.2.J.	•				
	70	F1 00									

. :

. . .

	796 797	NE2	GLN A	157 157 157	-0.638 1.086 -2.643	54.922 54.180 50.904	-23.635 -22.391 -22.872	1.00 1.00 1.00 1.00	249.69 249.69 176.07 176.07
2	798	C ·		157	-3.504	51.584 49.811	-23.430 -22,171	1.00	165.71
	799 2800	N	LEU A	158	-2.937 -4.320	49.375	-21.989	1.00	165.71
3	2801	CA	LEU A	158 158	-4.51 i	48.122	-22.809	1.00 1.00	232.32 232.32
	2802	CB	LEU A	158	-4.809	48.278	-24.317 -24.764	1.00	232.32
	2803	CG CD1	LEU A	158	-5.868	47.274 49.687	-24.663	1.00	232.32
	2804 2805	CD2	LEU A	158	-5.267 -4.642	49.105	-20.520	1.00	165.71 165.71
	2806	C	LEU A LEU A	158 158	-3.764	48.726	-19.741 -20.148	1.00 1.00	172.26
	2807	0 N	ASP A	159	-5.903	49,301 49,080	-18.772	1.00	172.26
	2808 2809	CA	ASP A	159	-6.321 -7.518	49.974	-18.431	1.00	159.32 159.32
15	2810	CB	ASP A	159 159	-7.259	51.435	-18.725	1.00 1.00	159.32
15	2811	CG	ASP A	159	-6.345	52.022	-18.103 -19.586	1.00	159.32
	2812	OD1 OD2	ASP A	159	-7.974	51.995 47.618	-18.556	1.00	172.26
	2813 2814	C	ASP A	159	-6.7€ -7.192	46.960	-19.479	1.00	172.26 165.86
20	2815	0	ASP A	159 160	-6.468	47.113	-17. 343 -17.016	1.00 1.00	165.86
	2816	N CA	TYR A	160	-6.826	45.741 44.810	-17.253	1.00	170.32
	2817 2818	CB	TYR A	160	-5.667 -5.121	44.887	-18.643	1.00	170.32 170.32
	2819	CG	TYR A	160 160	-3.121 -4.101	45.789	-18.959	1.00 1.00	170.32
25	2820	CD1	TYR A TYR A	160	-3.558	45.844	-20.241 -19.645	1.00	170.32
	2821	CE1 CD2	TYR A	160	-5.600	44.042 44.088	-20.937	1.00	170.32 170.32
	2822 2823	CE2	TYR A	160	-5.072 -4.046	44.988	-21.228	1.00 1.00	170.32
	2824	CZ	TYR A	160 160		45.018	-22.495 -15.586	1.00	165.86
30	2825	OH C	TYR A	160	-7.301	45.590 46.289	-14.675	1.00	165.86
	2826 2827	ŏ	TYR A	160		44.660	-15.410	1.00	140.66 140.66
	2828	N	GLU A GLU A	161 161		44.380	-14.119 -14 <i>.2</i> 72	1.00 1.00	201.20
	2829	CA CB	GLU A	161	-10.356	44.448 44.125	-13.044	1.00	201.20
35	2830 2831	CG	GLU A	161		44.551	-13.222		201.20 201.20
	2832	CD	GLU A	16 ⁻ 16 ⁻		44.011	-12.499 -14.076		201.20
	2833	OE1 OE2	GLU A	16	1 -12.920	45.434 42 <u>.</u> 987	-13.688		140.66
40	2834 2835	C	GLU A	16		42.095	-14.523	1.00	140.66 133.72
40	2836	ŏ	GLU A	16 16		42.815	-12.389	1.00 1 1.00	133.72
	2837	N	SER A SER A	16	2 -7.628	41.552	-11.84° -10.67°	`	153.53
	2838	CA CB	SER A	16		41.835 42.515	-9.61	6 1.00	153.53 133.72
45	2839 2840	ÖĞ	SER A		52 -7.366 52 -8.766	40.686	-11.34		133.72
7.	2841	Ç	SER A SER A		62 -9.852	41.187	-11.06 -11.22		190.14
	2842	0 N	GLU A	1	63 -8.517	39.386 38.488	-10.69	9 1.00	190.14
	2843 2844	CA	GLU A	\ 1	63 -9.539 63 -9.037	37.041	-10.70		249.69 249.69
50		CB	GLU A	\ 1	63 -8.981	36.372	-12.07 -12.6		249.69
	2846	CG	GLU A	•	63 -10.356	36.015 35.384	-11.9	28 1.00	249.69
	2847 2848	OE1	GLU /	A 1	163 -11.096 163 -10.694	35.284 38.462	-13.7		249.69 190.14
	2849	OE2	GLU /	•	163 -10.6 94 163 -9.764	38.962	-9.2 -8.6		190.14
5	5 2850	C	GLU A		163 -8.835	39.462	-8.7		116.57
	2851	0 N	PRO	A	164 -10.991	00 242	-9.4	112 1.00	155.66 116.57
	2852 2853	CD	PRO	• •	164 -12.208 164 -11.302	39.267	-7.3		
	2854	CA	PRO PRO		164 -12.814	4 39.411		394 1.00 263 1.00	155.66
(50 2855	CB CG	PRO		164 -13.20			325 1.00	116.57
	2856 2857	č	PRO	A	164 -10.82 164 -10.82			578 1.00	464 40
	2858	0	PRO LEU		164 -10.82 165 -10.44	38.735		.150 1.00 .122 1.00	151.49
	2859		1 1		165 -9.94	9 37.832		030 1.00	116.01
	65 2860 2861		LEU	Α	165 -8.41	~~ 001	-2	.995 1.00	
	2862	CG	LEU	Α	165 -7.71 165 -8.41	35.693	-2	.953 1.0 3.335 1.0	
	2863	3 CU		Ä	165 -6.24	44 36.924	· _	2.739 1.0	
	70 286 ⁴		LEU	A	165 -10.5	70 38.03	•		
	70 286	•							

	2866 2867	O N	LEU A ASN A ASN A	166 -10).651).996 1.583	39.156 36.932 36.988	-2.113 -0.779		151.49 136.62 136.62 179.00
	2868	CA	ASN A	166 -12	2.582	35.861	-0.576 -0.898	1.00	179.00
_	2869	CB CG	ASN A	166 -13	3.998	36.278	-0.835	1.00	179.00
	2870	OD1	ASN A	166 -1	4.338	37.458 35.305	-1.223	1.00	179.00
	2871 2872	ND2	ASN A	166 -1	4.839	36.890	0.307	1.00	138.62
	2873	C	ASN A		0.535 9.561	36.155	0.165	1.00	136.62
	2874	0	ASN A		0.741	37.619	1.401	1.00	136.70 136.70
10	2875	N	ILE A ILE A		9.795	37.605	2.521	1.00 1.00	129.99
_	2876	CA	ILE A		-8.857	38.814	2.472 3.694	1.00	129.99
	2877	CB CG2	ILE A	167	-7.953	38.809	1.209	1.00	129.99
	2876	CG1	ILE A		-8.012	38.756 39.934	1.059	1.00	129.99
15	287 <u>9</u> 2880	CD1	ILE A		-7.114 -0.406	37.621	3.867	1.00	136.70
15	2881	С	ILE A		10.496 11.317	38.494	4.126	1.00	136.70
	2882	0	ILE A		10.148	36.685	4.738	1.00	125.45 125.45
	2883	N	THR A THR A		10.808	36.66	6.016	1.00 1.00	120.45
	2884	CA CB	THR A		11.677	35.424	6.131 5.041	1.00	120.45
20	2885	OG1	THR A		-12.602	35.394	7.433	1.00	120.45
	2886 2887	CG2	THR A		-12.451	35.445 36.749	7.232	1.00	125.45
	2888	C	THR A	168	-9.910 -8.989	35.928	7.431	1.00	125.45
	2889	0	THR A	168 169	-10.194	37.757	8.050	1.00	104.30 104.30
25	2890	N	VAL A VAL A	169	-9.444	37.979	9.276	1.00 1.00	108.18
	2891	CA	VAL A VAL A	169	-9.061	39.471	9.422	1.00	108.18
	2892	CB CG1	VAL A	169	-8.798	39.826	10.864 8.602	1.00	108.18
	2893	CG2	VAL A	169	<i>-</i> 7.798	39.750 37.534	10.433	1.00	104.30
30	2894 2895	C	VAL A	169	-10.333	38.182	10.729	1.00	104.30
30	2896	ŏ	VAL A	169	-11.331 -9.972	36.416	11.069	1.00	193.03
	2897	N	ILE A	170	-9.972 -10.727	35.860	12.191	1.00	193.03 177.52
	2898	CA	ILE A ILE A	170 170	-10.701	34.321	12.132	1,00 1,00	177.52
	2899	CB	ILE A	170	-11.108	33.853	10.743 12.404	1.00	177.52
35	2900	CG2 CG1	ILE A	170	-9.291	33.800	12.422	1.00	177.52
	2901 2902	CD1	ILE A	170	-9.174	32.283 36.337	13.513	1.00	193.03
	2903	. C	ILE A	170	-10.133 -9.014	36.850	13.542	1.00	193.03
	2904	0	ILE A	170	-9.014	36.172	14.614	1.00	156.56 156.56
40	2905	N	LYS A	171 171	-10.335	36.621	15.921	1.00 1.00	223.67
	2906	CA	LYS A	171	-11.244	37.705	16.466 16.553	1.00	223.67
	2907	CB	LYS A	171	-12.675	37.247	16.449	1.00	223.67
	2908 2909	CD	LYS A	171	-13.639	38.495 39.423	17.548	1.00	223.67
45		CE	LYS A	171	-13.412	40.529	17.484	1.00	223.67
7.	2911	NZ	LYS A	171	-14.415 -10.169	35.507	16.984	1.00	156.56 156.58
	2912	Ç	LYS A LYS A		-9.911	35.776	18.164	1.00	229.93
	2913	0	LYS A NAG A		13.115	30.531	-12.704	1.00 1.00	229.93
	2914	C1 C2	NAG A		13.292	32.012	-13.027 -13.150		229.93
50		N2	NAG A	, 221		32.635 33.943	-12.957		229.93
	2916 2917	C7	NAG A	221		34.685	-12.679	1.00	229.93
	2918	07	NAG A			34.518	-13.100	1.00	229.93 229.93
	2919	C8	NAG A			32.185	-14.322		229.93
5	5 2920	C3	NAG A		•	33.560	-14.510		229.93
	2921	03	NAG A			31.386	-14.319 -15.66		229.93
	2922	C4 O4	NAG		1 15.903	31.411	-13.87		229.93
	2923 2924	C5	NAG	A 22		29.925 29.895	-12.62		229.93
•	50 2925	O5	NAG	A 22		29.114	-13.65	6 1.00	229.93
•	2926	C6	NAG			29.725	-12.70		229.93 249.69
	2927	Q6	NAG		· · ·	~4 000	-15.90		249.69
	2928	C1	NAG NAG	• •		32,101	-16.91		249.69
	2929	C2 N2	NAG	• • • • • • • • • • • • • • • • • • • •	<u>22</u> 17.769		-16.37 -16.20		249.69
1	65 2930	C7	NAG	A 2	22 18.879		-16.4		249.69
	2931 2932	07	NAG	A 2	22 20.003		-15.6	34 1.00	249.69
	2933	C8	NAG	· · ·	22 18.718 22 17.038		-18.2	36 1.00	
	2934	C3		· · ·	22 17.639 22 17.639		-19.2	17 1.00	249.03
	70 2935	O3	INAG	^ -	- :				

							-18.752	1.00	249.69
		C4	NAG A	222	16.979	30.571 30.501	-19.878	1.00	249.69
	2936 2937	04	NAG A	222	16.114	29.634	-17.646	1.00	249.69
	2937 2938	C5	NAG A	222	16.463	29.769	-16.459	1.00	249.69
	2939	O5 ·	NAG A	222	17.286	28.165	-18.038	1.00	249.69
5	2940	C6	NAG A	222	16.462 15.210	27.555	-17.749	1.00	249.69
,	2941	O6	NAG A	222 242	-3.871	18.493	-8.371	1.00	249.50
	2942	C1	NAG A	242	-3.270	18.370	-9.775	1.00	249.50 249.50
	2943	C2	NAG A NAG A	242	-1.860	18.040	-9.718	1.00 1.00	249.50
	2944	N2	NAG A	242	-1.426	16.919	-10.287 -10.862	1.00	249.50
10	2945	C7	NAG A	242	-2.178	16.128	-10.205	1.00	249.50
	2946	O7 C8	NAG A	242	0.063	16.621	-10.511	1.00	249.50
	2947	C3	NAG A	242	-3.480	19.691 19.600	-11.829	1.00	249.50
	2948 2949	03	NAG A	242	-2.951	20.019	-10.567	1.00	249.50
15	2950	C4	NAG A	242	-4.979 -5.159	21.345	-11.115	1.00	249.50
13	2951	O4	NAG A	242	-5.622	19.952	-9.158	1.00	249.50 249.50
	2952	C5	NAG A	242 242	-5.285	18.711	-8.481	1.00	249.50
	2953	O5	NAG A	242	-7.140	20.004	-9.2 3 5	1.00 1.00	249.50
	2954	C6	NAG A NAG A	242	-7.650	21.225	-8.725	1.00	249.69
20	2955	O6	NAG A	243	-5.905	21.444	-12.280 -12.441	1.00	249.69
	2956	C1 C2	NAG A	243	-6.423	22.875	-11.323	1.00	249.69
	2957	N2	NAG A	243	-7.258	23.262	-10.724	1.00	249.69
	2958 2959	C7	NAG A	243	-7.047	24.432 25.215	-11.062	1.00	249.69
25	2959	07	NAG A	243		24.787	-9.565	1.00	249.69
23	2961	C8	NAG A	243		22.971	-13.739	1.00	249.69
	2962	C3	NAG A	243		24,291	-13.913	1.00	249.69 249.69
	2963	03	NAG A	243 243		22.613	-14.888	1.00	249.69
	2964	C4	NAG A NAG A	243		22.760	-16.068	1.00 1.00	249.69
30	2965	04	NAG A	243		21.178	-14.681 -13.392	1.00	249.69
	2966	C5	NAG A	243		21.113	-15.727	1.00	249.69
	2967	O5 C6	NAG A	243		20.769	-15.679	1.00	249.69
	2968	06	NAG A	24		21.598 23.132	-17.256	1.00	249.69
35	2969 2970	C1	MAN A	24		22,291	-18.199	1.00	249.69
23	2971	C2	MAN A	24		22.309	-17.842	1.00	249.69
	2972	O2	MAN A	24 24		22.695	-19,610	1.00	249.69 249.69
	2973	C3	MAN A	24		21.811	-20.538	1.00 1.00	249.69
	2974	03	MAN A MAN A	24		24.155	-19.854		249.69
40		C4	MAN A	24		24.497	-21.200 -18.895		249.69
	2976	O4 C5	MAN A	24	14 -6.404	24.996	-17.507		249.69
	2977	O5	MAN A		44 -6.748	24.610 26.518	-19.137		249.69
	2978 2979	Č6	MAN A		44 -6.499	27.105	-18.519		249.69
4:		06	MAN A		44 -7.631 50 17.983	21.117	-1.207	7 1.00	249.69
→.	2981	C1	NAG A		50 17.983 50 19.036	440	-0.73		249.69 249.69
	2982	C2	NAG A	•	50 19.037		0.70		249.69
	2983	N2	NAG A		50 20.062	21.752	1.40		249.69
_	2984	C7	NAG A		250 21.042	21.214	0.87 2.92	-	249.69
5		O7 C8	NAG /	•	250 19.990		-1.35		249.69
	2986	C3	NAG	Ă i	250 18.721		-1.00		249.69
	2987 2988	03	NAG A	A :	250 19.730		-2.87		249.69
	2989	C4	NAG		250 18.61		-3.41	1.00	249.69
5	5 2990	Q4	NAG		250 18.193 250 17.613		-3.26		249.69 249.69
~	2991	C5	NAG	• •	250 17.61 250 17.98	6 21.032	-2.6		249.69
	2992	O5	NAG	• •	250 17.52	6 22.023	-4.79		249.69
	2993	C6	NAG NAG		250 16.88	7 20.775	-5.0		249.69
	2994	O6 C1	NAG		274 0.35	5 12.405			249.69
(50 2995	C2	NAG		274 -0.46		4-4		249.69
	2996 2997	N2	NAG	Α	274 0.42				249.69
	2998	C7	NAG		274 -0.07	400	4	1.00	249.69
	2999	07	NAG		274 -1.10 274 0.9		18.7	721 1.00	249.69
	65 3000	C8	NAG		274 0.9 274 -1.2		7 17.€		249.69 249.69
	3001	C3	NAG NAG		274 -2.1	30 13.222	2 18.4		
	3002				274 -2.1	17 11.38			
-	3003				274 -2.7	65 10.49	٠	768 1.00 901 1.00	
	70 3005				274 -1.2	21 . 10.59	D 15.		
	,0 300	, ,			•				

						44 505	15.017	1.00	249.69
	2006	O5	NAG A	274	-0.517	11.505 9.637	15.026	1.00	249.69
	3006 3007	C6	NAG A	274	-2.018 -1.206	9.058	14.010	1.00	249.69
	3008	O6	NAG A	274 335	5.793	44.302	-4.488	1.00	249.69
	3009	C1	NAG A	335	6.924	43.869	-3.512	1.00	249.69 249.69
5	3010	C2	NAG A NAG A	335	6.696	44.490	-2.220	1.00 1.00	249.69
	3011	N2	NAG A	335	6.442	43.744	-1.148 -1.175	1.00	249.69
	3012	C7 O7	NAG A	335	6.394	42.513	0.156	1.00	249.69
	3013	C8	NAG A	335	6.211	44.481 44.222	-3.983	1.00	249.69
10	3014 3015	ထိ	NAG A	335	8.352	43.421	-3.281	1.00	249.69
10	3016	03	NAG A	335	9.296 8.520	43.993	-5.483	1.00	249.69 249.69
	3017	C4	NAG A	335 335	9.821	44.401	-5.897	1.00	249.69
	3018	04	NAG A NAG A	335	7.450	44.802	-6. 20 5	1.00 1.00	249.69
	3019	C5 O5	NAG A	335	6.149	44.255	-5.895 -7.718	1.00	249.69
15	3020	C6	NAG A	335	7.609	44.762 46.071	-8.267	1.00	249.69
	3021 3022	06	NAG A	335	7.688	46.639	17.035	1.00	249.69
	3023	C1	NAG A	340	-3.087 -3.935	15,639	18.030	1.00	249.69
	3024	C2	NAG A	340 340	-4.856	44.975	17.311	1.00	249.69 249.69
20	3025	N2	NAG A NAG A	340	-4.995	43.695	17.659	1.00 1.00	249.69
	3026	C7	NAG A	340	-4.379	43.170	18.595 16.843	1.00	249.69
	3027	O7 C8	NAG A	340	-5.979	42.868	18.927	1.00	249.69
	3028	cs	NAG A	340	-4.707	46.820 46.110	19.924	1.00	249.69
25	3029 3030	O3	NAG A	340	-5.434	47.802	19.596	1.00	249.69
23	3031	C4	NAG A	340	-3.738 -4.485	48.790	20.299	1.00	249.69
	3032	04	NAG A	340 340	-2.841	48.473	18.533	1.00	249.69 249.69
	3033	C5	NAG A NAG A	340	-2.166	47.471	17.739	1.00 1.00	249.69
	3034	O5	NAG A	340	-1.761	49.371	19.114 18.103	1.00	249.69
30	3035	C6 O6	NAG A	340	-0.846	49.785	-1.870	1.00	221.62
	3036 3037	G1	NAG A	366	-16.179	35.618 34.642	-2.761	1.00	221.62
	3038	C2	NAG A	366	-16.600 -15.672	34.736	-3.871	1.00	221.62
	3039	N2	NAG A	366 366		33.944	-3.922	1.00	221.62 221.62
35	3040	C7	NAG A NAG A	366		33.096	-3.062	1.00 1.00	221.62
	3041	O7	NAG A	366		34.112	-5.114 -3.236	1.00	221.62
	3042	C8 C3	NAG A	366		34.981	-4.125	1.00	221.62
	3043 3044	og Og	NAG A	366		33.973 35.113	-2.065	1.00	221.62
40		C4	NAG A	366		35.683	-2.557	1.00	221.62 221.62
. +0	3046	04	NAG A	366 360		36.017	-0.964		221.62 221.62
	3047	- C5	NAG A NAG A	36	·	35.560	-0.585		221.62
	3048	O5	NAG A	36	.	36.056	0.304 1.205		221.62
4.6	3049	C6 O6	NAG A	36		37.042	-2.286		249.69
45	5 3050 3051	C1	NAG A	36		34.987 35.932	-2.38		249.69
	3052	C2	NAG A	36		37.053	-1.478		249.69
	3053	N2	A DAN			38.275	-1.96		249.69 249.69
	3054	C7	A DAN A DAN			38.512	-3.18		249.69
5	() 3055	. 07	NAG A		37 -22.101	39.407	-0.9 6 -2.05	·	249.69
	3056	C8 C3	NAG A		57 -23. 858	35.142 35.986	-2.16		249.69
	3057 3058	õ	NAG A	\ 3	67 -24.998	33.958	-3.03	1.00	249.69
	3059	C4	NAG A	•	67 -23.984 67 -25.101	33.153	-2.66		249.69 249.69
5	5 3060	04	NAG /	• -	67 -25.101 67 -22.694	33.108	-3.01	1.00	249.69
_	3061	C5	NAG / NAG /		67 -21.528	33.938	-3.25		249.69
	3062	O5 C6	NAG A		67 -22.696	32.031	-4.04 -5.0		249.69
	3063	O6	NAG		67 -21.707		23.8	• • • •	249.69
	3064 50 3065	CB	LYS	B 4	31.112	A 4 F D 7	23.2	60 1.00	249.69
•	3066	CG		_	4 31.172 4 31.232		24.3		249.69
	3067	CD		_	4 31.232 4 31.339		23.7		249.69 249.69
	3068	CE	LYS LYS		4 31.384	68.141	24.7		- 40 00
	3069		LYS	B	4 32.410	62.191	21.9 22.3		- 10 00
	65 3070		LYS	В	4 33.409		23.4		249.69
	3071 3072		LYS	В	4 31.07		22.	1.00	249.69
	3072		LYS	В	4 31.14 5 32.38			698 1.00	223.70
	3074	, N	PRO PRO	B	5 32.38 ³ 5 31.37		20.	128 1.00	195.56
	70 3075		PRU						

_		CA	PRO B	5	33.562	61.750	19.825 18.906	1.00 1.00	223.70 195.56
	076 077	CB	PRO B	5	33.387	60.550 60.498	18.724	1.00	195.56
	078	CG:	PRO B	5	31.904	63.077	19.060	1.00	223.70
	079	С	PRO B	5	33.598 32.576	63.741	18.895	1.00	223.70
	080	0	PRO B	5 6	34.780	63.472	18.605	1.00	208.07 208.07
3	3081	N	LYS B	6	34.916	64.713	17.858	1.00 1.00	245.96
	3082	CA CB	LYS B	6	35.357	65.849	18.783 18.074	1.00	245.96
	3083 3084	CG	LYS B	6	35.467	67.195 68.337	19.039	1.00	245.96
	3085	CD	LYS B	6	35.756	69.677	18.304	1.00	245.96
10	3086	CE	LYS B	6	35.816 35.973	70.834	19.231	1.00	245.96
	3087	NZ	LYS B LYS B	6 6	35.920	64.543	16.721	1.00	208.07 208.07
	3088	C	LYS B LYS B	6	37.122	64.371	16.946	1.00 1.00	211.91
	3089	0 N	VAL B	7	35.414	64.603	15.497 14.312	1.00	211.91
15	3090	CA	VAL B	7	36.245	64.443 64.356	13.053	1.00	105.28
	3091 3092	СВ	VAL B	7	35.379	63.818	11.881	1.00	105.28
	3093	CG1	VAL B	7	36.218 34.151	63.495	13.325	1.00	105.28 211.91
	3094	CG2	VAL B VAL B	7 7	37.258	65.565	14.107	1.00	211.91
20	3095	C	VAL B	7	36.903	66.741	14.033	1.00 1.00	208.76
	3096	O N	SER B	8	38.524	65.185	14.009 13.797	1.00	208.76
	3097 3098	CA	SER B	8	39.599	66.141 65.846	14.770	1.00	216.01
	3099	CB	SER B	8	40.749	64.465	14.777	1.00	216.01
25	3100	OG	SER B	8	41.085 40.084	66.033	12.348	1.00	208.76
20	3101	Ç	SER B	8 8	39.830	65.031	11.685	1.00	208.76 194.89
	3102	0	SER B LEU B	9	40.767	67.061	11.853	1.00 1.00	194.89
	3103	N CA	LEU B	9	41.278	67.030	10.487 9.599	1.00	159.88
20	3104	CB	LEU B	9	40.528	68.017	9,401	1.00	159.88
30	3105 3106	ČĞ	LEU B	9	39.017	67.914 68.762	8.190	1.00	159.88
	3107	CD1	LEU B	9	38.658 38.575	66.489	9.175	1.00	159.88
	3108	CD2	LEU B	9	42.760	67.363	10.413	1.00	194.89 194.89
	3109	Ç	LEV B LEV B	8	43.318	67.981	11.315	1.00 1.00	186.22
35	3110	0 N	ASN B	10	43.390	66.956	9.319 9.113	1.00	186.22
	3111 3112	CA	ASN B	10		67.229 66.253	9.914	1.00	231.85
	3113	CB	ASN B	10		66.704	10.015	1.00	231.85
	3114	CG	ASN B	10		67.753	10.592	1.00	231.85 231.85
40	3115	OD1	ASN B	10 10		65.921	9.445	1.00 1.00	186.22
	3116	ND2	ASN B	10	·	67.123	7.638 7.059		186.22
	3117	CO	ASN B	10	45.137	66.030	6.991	1.00	188.99
	3118 3119	Ň	PRO B	11		68.262 68.247	5.571		219.87
45	3120	CD	PRO B	1		69.622	7.539	1.00	188.99
75	3121	CA	PRO B	1		70.458	6.284		219.87 219.87
	3122	CB	PRO B PRO B	i		69.52 6	5.431		188.99
	3123	C C	PRO B		1 44.336	70.101	8.267 8.188	_	188.99
50	3124 3125	ŏ	PRO B		1 43.282	69.480 71.222	9.00	-	172.73
30	3126	Ň	PRO B	1	2 44.443	71.989	9.31	1 1.00	135.97
	3127	CD	PRO B		2 45.661 2 43.290	71.755	9.73	9 1.00	172.73 135.97
	3128	CA	PRO B		12 43.290 12 43.920	72.837	10.62	3 1.00	135.97
	3129	CB CG	PRO B		2 45.37s	72.451	10.70 8.74		172.73
55		C	PRO B		12 42 <i>.2</i> 74		9.01		172.73
	3131 3132	ŏ	PRO E	3	12 41.079		7.59		154.67
	3133	N	TRP		13 42.788 13 42.024		6.50	3 1.00	154.67
	3134	CA	TRP	3	13 42.024 13 42.952		5.30	00 1.00	165.26 165.26
60) 3135	CB	TRP 1	-	13 44.249	74.215	5.65		165.26
	3136	CG CD2	TRP	_	13 44.455	75.194	6.65 6.65		165.26
	3137	CE2	TRP	B	13 45.818		7.6		165.26
	3138 3139	CE3	TRP	В	13 43.612		5.0		165.26
6	5 3140	CD1	TRP	B	13 45.46		5.6	68 1.00	
J	3141	NE1			13 46.419 13 46.35	400	7.5		
	3142	CZ2		B	13 44.14	6 76.753	8.4		
	3143	CZ3 CH2		B	13 45.50	6 77.080		1.00 1.00 1.00	
-	3144 70 3145	C	TRP	В	13 40.84	0 · 72.520	0.0	,	
•	, J 170	_							

					•		r 602	1.00	154.67
		_	TRP B	13	41.023	71.414	5.593 6.265	1.00	126.91
	146	0	ASN B	14	39.627	73.038	5.885	1.00	126.91
	147	N CA	ASN B	14	38.416	72.290 72.308	7.035	1.00	191.01
	148	CB .	ASN B	14	37.397	72.306 73.687	7.331	1.00	191.01
3	149	CG	ASN B	14	36.877	74.604	7.635	1.00	191.01
	1150 3151	OD1	ASN B	14	37.643	73.848	7.246	1.00	191.01
	3152	ND2	ASN B	14	35.564 37.778	72.796	4.590	1.00	126.91 126.91
	3153	C	ASN B	14 14	36.595	72.577	4.336	1.00 1.00	109.47
	3154	0	ASN B ARG B	15	38.606	73.477	3.799 2.509	1.00	109.47
	3155	N.	ARG B	15	38.240	74.033	2.571	1.00	119.97
	3156	CA	ARG B	15	38.096	75.576	3.671	1.00	119.97
	3157	CB CG	ARG B	15	37.202	76.153 77.677	3.482	1.00	119.97
	3158	CD	ARG B	15	37.010	78.008	2.444	1.00	119.97
15	3159 3160	NE	ARG B	15	36.034 36.135	79.040	1.615	1.00	119.97 119.97
13	3161	CZ	ARG B	15 15	37.176	79.846	1.693	1.00 1.00	119.97
	3162	NH1	ARG B	15	35.187	79.273	0.715	1.00	109.47
	3163	NH2	ARG B ARG B	15	39.432	73.688	1.616 1.689	1.00	109.47
	3164	C	ARG B	15	40.462	74.353	0.769	1.00	122.07
20	3165	O N	ILE B	16	39.307	72.675 72.294	-0.072	1.00	122.07
	3166	CA	ILE B	16	40.431	70.905	0.303	1.00	121.17
•	3167 3168	CB	ILE B	16	40.914	70.954	1,608	1.00	121.17 121.17
	3169	CG2	ILE B	16	41.691 39.708	69.975	0.377	1.00	121.17
25	3170	CG1	ILE B	16 16	40.058	68.526	0.495	1.00	122.07
23	3171	CD1	ILE B ILE B	16	40.206	72.279	-1.571	1.00 1.00	122.07
	3172	C	ILE B ILE B	16	39.087	72.146	-2.041 -2.314		169.19
	3173	0	PHE B	17	41.299	72.390	-3.770		169.19
-00	3174	N CA	PHE B	17		72.361 72.815	-4.351		156.59
30	3175	CB	PHE B	17		74,285	-4.609	1.00	156.59
	3176 3177	ČĞ	PHE B	17		74,960	-4.420		156.59 156.59
	3178	CD1	PHE B	17 17		74.990	-5.076		158.59
	3179	CD2	PHE B	17		76.315	-4.690		156.59
35	3180	CE1	PHE B PHE B	17		76.350	-5.349 -5.15	•	156.59
	3181	CE2	PHE B	1	7 42.886	77.013	-3.13 -4.25	·	169.19
	3182	CZ C	PHE B	1		70.947 70.006	-3.46	0 1.00	169.19
	3183 3184	ŏ	PHE B	1			-5.57	5 1.00	133.30
40	3185	Ň	LYS B	1		-0 -04	-6.20		133.30 237.07
70	3186	CA	LYS B		8 40.573 8 39.922	69.777	·7.57		237.07
	3187	CB	LYS B Lys b		8 39.500	68.537	-8.33 -9.58		237.07
	3188	cg	LYS B		18 38.720		-10.44		237.07
	3189	CE	LYS B		18 38.347		-11.0		237.07
45	3190	NZ	LYS B		18 39.539		-6.3	63 1.00	133.30
	3191 3192	Ċ	LYS B		18 41.85° 18 42.86°		-6.8		133.30 182.54
	3193	0	LYS			440	-5.8		182.54
	3194	N	GLY E		19 41.79 19 42.94		-6.0		182.54
50	3195	CA	GLY E		19 43.82	3 66.498	-4.7 -4.7	·	182.54
	3196	C	GLY I	á	19 44.70		-3.8	- 400	116.49
	3197	0 N	GLU !	В	20 43.59	~~ 404		606 1.00	116.49
	3198	CA	GLU !	В	20 44.39			920 1.00	185.38
5	3199 5 320 0	CB	GLU	В	20 44.4	010	-2.1	822 1.00	185.38 185.38
,	3201	ÇG	GLU	В	20 44.4	=4 000		047 1.00	405.00
	3202	CD	GLU		20 43.5	13 71 <i>.</i> 585		288 1.00 205 1.00	405.00
	3203	OE1			20 45.4	33 72.125		.205 1.00 .622 1.00	
	3204	OE2	GLU	В	20 43.9	48 66.330		.729 1.00	116.49
•	50 3205	CO	GLU	В	20 42.8			.669 1.00	130.57
	3206 3207	N	ASN	В	21 44.8	04.044	'	.300 1.00	
	3207 3208	CA	ASN	В	21 44.4 21 45.4	20 701	i	353 1.00	
	3209	CB		В		00.40/	2 -0	0.992 1.0	242.40
	65 3210	CG		D D		414 63.34	7	2.004 1.0 0.980 1.0	-40.40
	3211	OD				420 63.38·	•	0.980 1.0 1.730 1.0	
	3212		2 ASN ASN		21 44.	229 65.43	•	2.194 1.0	0 130.57
	3213		ASN	В		.972 66.30 243 64.86	•	2.428 1.0	
	70 3214 70 3215	T 61	VAL		22 43	.243 64.86	~		
	10 321	-							

1 a - 4 - 24

			_		42.933	65.242	3.810	1.00	161.15
	3216	CA	VAL B	22	42.833	66.157	3.876	1.00	160.53
	3217	CB	VAL B	22 22	40,447	65.365	3.549	1.00	160.53
	3218	CG1.	VAL B VAL B	22	41.584	66.778	5.249	1.00	160.53 161.15
_	3219	ÇG2	VAL B	22	42.633	64.002	4.652	1.00 1.00	161.15
5	3220	C	VAL B	22	42.062	63.035	4,141	1.00	186.22
	3221	0 N	THR B	23	42.985	64.041	5.940 6.849	1.00	186.22
	3222	CA	THR B	23	42.771	62.898	7.478	1.00	249.25
	3223	CB	THR B	23	44.108	62.440	6.448	1.00	249.25
10	3224 3225	OG1	THR B	23	45.086	62.250 61.136	8.238	1.00	249.25
10	3226	CG2	THR B	23	43.919	63.173	8.004	1.00	186.22
	3227	С	THR B	23	41.804 42.015	64,109	8.783	1.00	186.22
	3228	0	THR B	23 24	40.764	62.345	8.132	1.00	183.26
	3229	N .	LEU B	24	39.782	62.522	9.208	1.00	183.26 177.01
15	3230	CA	LEU B LEU B	24	38.339	62.398	8.677	1.00 1.00	177.01
	3231	CB CG	LEU B	24	37.949	62.842	7.258	1.00	177.01
	3232	CD1	LEU B	24	36.435	62.918	7.183 6.910	1.00	177.01
	3233	CD2	LEU B	24	38.553	∈ 190 61.501	10.329	1.00	183.26
20	3234 3235	C	LEU B	24	39.974	60.321	10.162	1.00	183.26
20	3236	Ö	LEU B	24	39.661	61.965	11.472	1.00	238.46
	3237	N	THR B	25	40.476 40.717	61.111	12.636	1.00	238.46
	3238	CA	THR B	25 25	42.027	61.517	13.351	1.00	207.80
	3239	CB	THR B	25	43.116	61.448	12.424	1.00	207.80
25	3240	OG1	THR B	25	42.312	60.594	14.527	1.00	207.80 238.46
	3241	CG2	THR B	25	39.562	61.234	13.632	1.00 1.00	238.46
	3242	CO	THR B	25	39.133	62.342	13.949 14.126	1.00	203.48
	3243	N	CYS B	26	39.069	60.099	15.088	1.00	203.48
20	3244 3245	ČA	CYS B	26	37.965	60.098	16,500	1.00	203.48
30	3245 3246	Č.	CYS B	26	38.484	60.356 59.880	16.861	1.00	203.48
	3247	Ō	CYS B	26	39.563 37.227	58.767	15.036	1.00	181,40
	3248	СВ	CYS B	26	35.662	58.718	15.964	1.00	181.40
	3249	SG	CYS B ASN B	26 27	37,708	61.100	17.294	1.00	249.69 249.69
35	3250	N	asn b Asn b	27	38.087	61.472	18.666	1.00 1.00	249.69
	3251	CA CB	ASN B	27	36.876	61.388	19.608	1.00	249.69
	3252	CG	ASN B	27	37.148	62.023	20.969 21.060	1.00	249.69
	3253 3254	OD1	ASN B	27	37.644	63.155	22.033	1.00	249.69
40		ND2	ASN B	27	36.820	61.299 60.677	19.254	1.00	249.69
40	3256	C	ASN B	27	39.259	59.605	19.837	1.00	249.69
	3257	0	ASN B	27		61.234	19.090	1.00	244.48
	3258	N	GLY B	28 28		60.619	19.577	1.00	244.48 244.48
	3259	ÇA	GLY B	28		61.439	19.026	1.00	244.48
45		C	GLY B	28		61.561	17.809	1.00 1.00	249.69
	3261	0 N	ASN B	29	43.638	62.008	19.912	1.00	249.69
	3262 3263	ČA	ASN B	29		62.853	19.497 20.698	1.00	249.69
	3264	CB	ASN B	29		63.688 64. 79 7	20.295	1.00	249.69
50		ĊĠ	ASN B	29		65.073	19.106	1.00	249.69
٠,	3266	OD1	ASN B	2		65.444	21.293	1.00	249.69
	3267	ND2	ASN B		45.090	62.076	18.865		249.69
	3268	Ç	ASN B ASN B	2	9 48.375	62.412	17.757		249.69 249.69
_	3269	Ö	ASN B		0 46.412	61.034	19.543		249.69
5	5 3270	N CA	ASN B		0 47.543	60.279	19.017 19.881		249.69
	3271	CB	ASN E		0 48.783		19.831		249.69
	3272 3273	CG	ASN E		30 49.224		20.869		249.69
	3274	OD1	ASN E	3 3	30 49.500	~~ =~ 4	18.62		249.69
6	0 3275	ND2	ASN E	-	30 49.301		18.86	4 1.00	249.69
•	3276	С	ASN I		30 47, 3 41 30 47, 2 89		17.73	6 1.00	249.69
	3277	0	ASN				19.98	5 1.00	249.69 249.69
	3278	N	PHE		31 47.227 31 47.068		19.93		249.69
•	3279	CA	PHE PHE	R	31 48.220	55.917	20.70		249.69
(65 3280	CB CG	PHE		31 49.60	1 56.344	20.23		249.69
	3281	CD1			31 50.15		20.66 19.34		249.69
	3282 3283	CD2	PHE	В	31 50.33		20.20		249.69
	3284	CE1	PHE	В	31 51.40		18.88		249.69
	70 3285	CE2		В	31 51.58	8 . 55.807			

			PHE B	31 ⁻	52,121	57.182	19.313	1.00 1.00	249.69 249.69
	3286	cz		31	45.718	56.071	20.433	1.00	249.69
	3287	Ç.	PHE B	31	45.325	56.313	21.577	1.00	249.69
	3288	O .	PHE B	32	45.027	55.341	19.556 19.859	1.00	249.69
_	3289	N CA	PHE B	32	43.717	54.761	18.875	1.00	249.69
5	3290	CB	PHE B	32	42.670	55.314	19.304	1.00	249.69
	3291	CG	PHE B	32	41.238	55.081	20.443	1.00	249.69
	3292 3293	CD1	PHE B	32	40.722	55.709 54.237	18.565	1.00	249.69
	3294	CD2	PHE B	32	40.404	54.237 55.4 9 9	20.835	1.00	249.69
10	3295	CE1	PHE B	32	39.398	54.022	18.950	1.00	249.69
10	3296	CE2	PHE B	32	39.081	54.655	20.087	1.00	249.69
	3297	CZ	PHE B	32	38.578	53.220	19.785	1.00	249.69
	3298	C ,	PHE B	32	43.771 44.746	52.646	19.285	1.00	249.69
	3299	0	PHE B	32	42.714	52.559	20.259	1.00	249.69
15	3300	N	GLU B	33 33	42.688	51.104	20.273	1.00	249.69
	3301	CA	GLU B	33	42.563	50.633	21.724	1.00	249.69 249.69
	3302	CB	GLU B	33	42.965	49.185	21.932	1.00	249.69
	3303	CG	GLU B GLU B	33	44.299	48.858	21.285	1.00	249.69
	3304	CD	GLU B	33	45.257	49.641	21.471	1.00	249.69
20	3305	OE1	GLU B	33	44.389	47.819	20.593	1.00 1.00	249.69
	3306	OE2	GLU B	33	41.644	50.384	19.409	1.00	249.69
	3307	C	GLU B	33	41.991	49.478	18.645	1.00	249.69
	3308	0	VAL B	34	40.375	50.773	19.532	1.00	249.69
	3309	N	VAL B	34	39.290	50.129	18.784	1.00	247.84
25	3310	CA	VAL B	34	37.920	50.767	19.158	1.00	247.84
	3311	CB	VAL B	34	36.794	50.060	18.427 20.661	1.00	247.84
	3312	CG1 CG2	VAL B	34	37.698	50.681	17.252	1.00	249.69
	3313		VAL B	34	39.448	50.119	16.663	1.00	249.69
	3314	C O	VAL B	34	40.059	51.023	16.627	1.00	249.69
30	3315	Ň	SER B	35	38.895	49.077	15.175	1.00	249.69
	3316	CA	SER B	35	38.934	48.909	14.806	1.00	240.73
	3317	CB	SER B	35	39.389	47.500	15.104	1.00	240.73
	3318	og	SER B	35	38.373	46.555	14.625	1.00	249.69
25	3319	č	SER B	35	37.529	49.126	13.412	1.00	249.69
35	3320 3321	ŏ	SER B	35	37.305	49.055 49.371	15.533	1.00	249.69
	3322	Ň	SER B	36	36.583	49.611	15.162	1.00	249.69
	3323	ČA	SER B	36	35.186	48.825	16.081	1.00	249.69
	3324	СВ	SER B	36	34.233	49.372	17.391	1.00	249.69
40		OG	SER B	36	34.184	51.108	15.231	1.00	249.69
40	3326	C	SER B	36	34.857	51.639	16.278	1.00	249.69
	3327	0	SER B	36	34.462 35.037	51.780	14.102	1.00	249.69
	3328	N	THR B	37	34,765	53.198	14.004	1.00	249.69
	3329	CA	THR B	37	36.076	53.989	13.773		184.28
45	3330	CB	THR B	37 37		53.759	14.866	1.00	184.28 184.28
•••	3331	OG1	THR B	37		55.477	13.679		184.26 249.69
	3332	CG2	THR B	37		53.375	12.823		249.69
	3333	Ç	THR B	37		52.726	11.782		236.74
	3334	0		38		54,236	12.988		236.74
5	0 3335	N	LYS B	38		54.464	11.930	1.00	245.72
	3336	CA	LYS B	38		54.378	12.519		245.72
	3337	CB	LYS B	31		53.037	13.196		245.72
	3338	ÇG	LYS B			52.984	13.8.1		245.72
_	3339	CD.	LYS E	3		51.615	14.41		245.72
5	5 3340	CE	LYS B			51.521	14.99	_	236.74
	3341	NZ	LYS B			55.806	11.22 11.84		236.74
	3342	CO	LYS B		8 32.415	56.797	9.92		197.18
	3343	N	TRP B	_	g 31.805	55.821	9.52		197.18
,	3344	CA	TRP E		9 31.946	57.042	8.18		174.88
,	3345	CB	TRP E		39 33.131	56.937	8.84		174.88
	3346	õ	TRP E		39 34.474		9.70		174.88
	3347	CD2		3 3	39 35.068		9.97		174.88
	3348	CE2			39 36.391		10.27		174.88
	3349	CE3			39 34.614		8.6		174.88
'	65 3350	CD1			39 35.433		9.3	• • • • • •	174.88
	3351	NE1	TRP	В	39 36.589		9.3 10.7		174.88
	3352 3353	CZ2	TRP	В	39 37.26		11.0		174.88
	3353	CZ3	TRP	В	39 35.48		44.0		174.88
	70 3355	CH2			39 36.79	8 59.357			
	,, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,				•				

			_		00.007	57.211	8.335	1.00	197.18
	3356	С	TRP B	39-	30.667 30.215	56.251	7.708	1.00	197.18
	3357	0	TRP B	39 40	30.213	58.413	8.348	1.00	196.05
	3358	N	PHE B PHE B	40	28.848	58.653	7.609	1.00	196.05
_	3359	CA CB	PHE B	40	27.674	58.878	8.572	1.00 1.00	216.66 216.66
5	3360	CG	PHE B	40	27.425	57.738	9.528 10.679	1.00	216.66
	3361 3362	CD1	PHE B	40	28.199	57.602	9.297	1.00	216.66
	3363	CD2	PHE B	40	26.396	56.824 56.578	11.590	1.00	216.66
	3364	CE1	PHE B	40	27.951 26.139	55.800	10.194	1.00	216.66
10	3365	CE2	PHE B	40 40	26.135	55.674	11.345	1.00	216.66
	3366	CZ	PHE B	40	28.896	59.825	6.616	1.00	196.05 196.05
	3367	C	PHE B	40	28.336	60.888	6.877	1.00 1.00	132.87
	3368	O N	HIS B	41	29.552	59.613	5.476 4.418	1.00	132.87
15	3369 3370	CA	HIS B	41	29.665	60.618	3.315	1.00	148.70
13	3370	СВ	HIS B	41	30.576	60.097 61.067	2.198	1.00	148.70
	3372	CG	HIS B	41	30.772 30.886	60.877	0.864	1.00	148.70
	3373	CD2	HIS B	41 41	30.860	62.416	2.414	1.00	148.70
	3374	ND1	HIS B HIS B	41	31.166	63.019	1.259	1.00	148.70 148.70
20	3375	CE1 NE2	HIS B HIS B	41	31.135	62.108	0.304	1.00 1.00	132.87
	3376	C	HIS B	41	28.311	60.975	3.804 2.996	1.00	132.87
	3377	ŏ	HIS B	41	27.783	60.210	4.163	1.00	209.30
	3378 3379	Ň	ASN B	42	27.777	62.147 62.614	3.684	1.00	209.30
25	3380	CA	ASN B	42	26.467	62.546	2.148	1.00	240.31
20	3381	CB	ASN B	42	26.371 27.092	63.700	1.461	1.00	240.31
	3382	CG	ASN B	42 42	28.241	63.989	1.789	1.00	240.31
	3383	OD1	ASN B ASN B	42	26.427	64.350	0.505	1.00	240.31 209.30
	3384	ND2	ASN B	42	25.375	61.745	4.316	1.00 1.00	209.30
30	3385	C	ASN B	42	24.271	61.613	3.774 5.475	1.00	171.14
	3386 3387	Ň	GLY B	43	25.695	61.168 60.306	6.176	1.00	171.14
	3388	CA	GLY B	43	24.758	58.836	5.841	1.00	171.14
	3389	C	GLY B	43	24.985 24.963	57.969	6.717	1.00	171.14
35	3390	0	GLY B	43 44	25.211	58.563	4.560	1.00	214.62
	3391	N	SER B SER B	44	25.444	57.207	4.071	1.00	214.62 249.69
	3392	CA	SER B	44	25.676	57.228	2.555	1.00 1.00	249.69
	3393	CB OG	SER B	44	24.567	57.774	1.864 4.733	1.00	214.62
40	3394 3395	C	SER B	44		56.559	4.657	1.00	214.62
40	3396	ŏ	SER B	44		57.088 55.404	5.359	1.00	180.32
	3397	N	LEU B	45		54.713	6.008	1.00	180.32
	3398	CA	LEU B	. 45 45		53.361	6.558	1.00	218.81
	3399	CB	LEU B LEU B	45		52.573	7.318	1.00	218.81 218.81
45		CG CD1	LEU B	45		53.429	8.432		218.81
	3401	CD2	LEU B	4	27.568	51.300	7.883 5. 03 0		180.32
	3402 3403	C	LEU B	4		54.516 54.279	3.819		180.32
	3404	Ō	LEU B	4		54.379 54.517	5.565		248.98
50	3405	N	SER B	. 4		54,357	4.757		248.98
	3406	CA	SER B SER B	. 4		55.405	5.149		249.38 249.38
	3407	OG CB	SER B		6 33.322	55.338	4.301		248.98
	3408	C	SER B		6 31.747	52.967	4.898 5.773		248.98
5	3409 5 3410	ŏ	SER B	4	6 31.351	52.195	4.04		249.69
ر	3411	N	GLU B		7 32.72	52.670 51.365	4.03	-	249.69
	3412	CA	GLU B		7 33.387 7 33.757	50.996	2.59	3 1.00	249.69
	3413	СВ	GLU B		··	50.869	1.67		249.69
	3414	ca	GLU B GLU B		17 32.553 47 32.945	50.524	0.25		249.69 249.69
6	0 3415	CD	GLU E		47 33.631	51.350	-0.38		249.69 249.69
	3416	OE1 OE2	GLU E	-	47 32.572		-0.21 4.92		249.69
	3417 3418	C	GLU E	3	47 34.618	51.211	4.92 5.13		249.69
	3418 3419	ŏ	GLU E	3	47 35.099		5.44		184.88
1	55 3420	Ň	GLU (3	48 35.139		6.3	16 1.00	184.88
	3421	CA	GLU 1		48 36.297 48 37.110		6.2	88 1.00	208.21
	3422	CB	GLU		48 37.110 48 38.293		7.2		208.21 208.21
	3423	CG	GLU GLU	B	48 39.366	52.513	6.9		208.21
	3424	CD OE1			48 40.08		5.9	37 1.00	200.21
	70 3425	V L1							

	0400	OE2	GLU B	48 .	39.493	51.517	7.685	1.00	208.21
	3426 3427	C	GLU B	48	35.834	51.929	7.738	1.00	184.88
	3428	ŏ	GLU B	48	34.687	52.213	8.104	1.00	184.88
	3429	Ň	THR B	49	36.731	51.348	8.530	1.00	237.20
5	3430	CA	THR B	49	36.443	51.003	9.917	1.00	237.20
	3431	СВ	THR B	49	36.348	49.477	10.090 9.586	1.00 1.00	231.33
	3432	OG1	THR B	49	37.542	48.864 48.933	9.336	1.00	231.33 231.33
	3433	CG2	THR B THR B	49 49	35.144 37.540	51,551	10.829	1.00	237.20
10	3434	C	THR B THR B	49	37.303	51.819	12.006	1.00	237.20
10	3435 3436	Ň	ASN B	50	38.739	51.713	10.278	1.00	222.02
	3437	ĊA	ASN B	50	39.863	52.246	11.036	1.00	222.02
	3438	СВ	ASN B	50	41.101	52.350	10.132	1.00	245.81
	3439	CG	ASN B	50	42.369	52.650	10.910	1.00 1.00	245.81 245.81
15	3440	OD1	ASN B	50	42.309	53.119 52.400	12.045 10.299	1.00	245.81
	3441	ND2	ASN B	50 50	43.520 39.447	53.636	11.531	1.00	222.02
	3442 3443	C	ASN B ASN B	50	38.625	54.290	10.901	1.00	222.02
	3444 3444	N	SER B	51	40.004	54.089	12.651	1.00	208.27
20	3445	ĊA	SER B	51	39.652	55.405	13.176	1.00	208.27
	3446	CB	SER B	51	40.219	55.590	14.590	1.00	249.69
	3447	OG	SER B	51	41.624	55.785	14.565	1.00 1.00	249.69 208.27
	3448	Ç	SER B	51	40.135	56.555 57.690	12.276 12.416	1.00	208.27
25	3449	0	SER B	51 52	39.672 41.059	56.265	11.360	1.00	249.32
25	3450	N CA	SER B SER B	52 52	41.588	57.283	10.446	1.00	249.32
	3451 3452	CB	SER B	52	43.125	57.283	10.456	1.00	193.43
	3453	OG	SER B	52	43.642	57.584	11.741	1.00	193.43
	3454	Ċ	SER B	52	41.106	57.076	9.014	1.00	249.32
30	3455	0	SER B	52	41.596	56.199	8.299	1.00	249.32 187.33
	3456	N	LEU B	53	40.147	57.895 57.820	8.601 7.255	1.00 1.00	187.33
	3457	CA	LEU B	53 53	39,601 38,107	57.620 58.131	7.283	1.00	113.92
	3458	CB CG	LEU B	53 53	37.410	58.539	5.975	1.00	113.92
35	3459 3460	CD1	LEU B	53	37.839	57.637	4.810	1.00	113.92
))	3461	CD2	LEU B	53	35.889	58.503	6.185	1.00	113.92
	3462	С	LEU B	53	40.310	58.794	6.331	1.00	187.33
	3463	0	LEU B	53	40.085	60.010	6.397 5.467	1.00 1.00	187.33 190.27
40	3464	N	ASN B	54	41.169	58.261 59.112	4.547	1.00	190.27
40	3465	CA	ASN B ASN B	54 54	41.899 43.209	58.458	4.126	1.00	248.26
	3466 3467	CB CG	ASN B	54	44.214	58.414	5.254	1.00	248.26
	3468	OD1	ASN B	54	44.519	59.432	5.876	1.00	248.26
	3469	ND2	ASN B	54	44.737	57. 23 2	5.525	1.00	248.26
45	3470	С	ASI: B	54	41.096	59.481	3.320	1.00	190.27 190.27
	3471	0	ASN B	54	40.134	58.800	2.957 2.700	1.00 1.00	195.13
	3472	N	ILE B	55 55	41.515 40.900	60.580 61.127	1.503	1.00	195.13
	3473 3474	CA CB	ILE B	55 55	40.101	62.413	1.829	1.00	126.27
50	3475	CG2	ILE B	55	39.946	63.268	0.581	1.00	126.27
50	3476	CG1	ILE B	55	38.743	62.032	2.431	1.00	126.27
	3477	CD1	ILE B	55	37.857	63.206	2.786	1.00	126.27
	3478	С	ILE B	55	42.017	61.473	0.540	1.00 1.00	195.13 195.13
	3479	0	ILE B	5 5	42.836	62.346 60.789	0.8 2 5 -0.594	1.00	178.85
55	3480	N OA	VAL B	56 56	42.057 43.099	61.058	-1.569	1.00	178.85
	3481 3482	CA CB	VAL B VAL B	56	43.587	59.773	-2.227	1.00	249.69
	3483	CG1	VAL B	56	44.960	60.002	-2.841	1.00	249.69
	3484	CG2	VAL B	56	43.642	58.662	-1.189	1.00	249.69
60	3485	С	VAL B	56	42.580	62.012	-2.630	1.00	178.85
	3486	0	VAL B	56	41.612	62.729	-2.376	1.00 1.00	178.85 192.84
	3487	N	ASN B	57	43.217	62.025 62.923	-3.804 -4.895	1.00	192.84
	3488	CA	ASN B	57 57	42.832 43.085	62.261	-6.239	1.00	201.25
65	3489 3490	CB CG	asn b Asn b	57	44.560	62.119	-6.530	1.00	201.25
UJ.	3491	OD1	ASN B	57	45.309	63.090	-6.446	1.00	201.25
	3492	ND2	ASN B	57	44.988	60.908	-6.875	1.00	201.25
	3493	C	ASN B	57	41.397	63.405	-4.791 5.067	1.00	192.84
~~	3494	0	ASN B	57	40.470	62.757	-5.267 -4.151	1.00 1.00	192.84 127.65
70	3495	N	ALA B	58	41.253	64.565	-4.151	1.00	127.00

3496 CA 3497 CB 3498 C 3499 O	ALA B 58 ALA B 58 ALA B 58 ALA B 58 LYS B 58	3 40.256 3 39.029 3 39.244	65.227 66.555 65.436 66.294 64.658	-3.870 1.00 -3.201 1.00 -5.041 1.00 -5.891 1.00 -5.060 1.00	127.65 133.74 127.65 127.65 124.63 124.63
5 3500 N 3501 CA 3502 CB 3503 CG	LYS B 55 LYS B 55 LYS B 55	9 36.946 9 36.504 9 37.632	64.744 63.344 62.491 61.069	-6.109 1.00 -6.550 1.00 -7.108 1.00 -7.421 1.00	240.20 240.20 240.20
3504 CD 10 3505 CE 3506 NZ 3507 C	LYS B 5 LYS B 5 LYS B 5	9 38.354 9 37.959 9 35.778 9 35.423	60.214 58.816 65.493 65.278	-7.901 1.00 -8.237 1.00 -5.511 1.00 -4.355 1.00 -6.301 1.00	240.20 240.20 124.63 124.63 146.51
3508 O 3509 N 15 3510 CA 3511 CB	PHE B 6	35.188 60 34.064 60 33.350 60 34.189	66.378 67.179 67.788 68.770	-5.839 1.00 -7.049 1.00 -7.815 1.00	146.51 206.05 206.05 206.05
3513 CD1 3514 CD2 20 3515 CE1	PHE B PHE B PHE B	60 33.968 60 35.193 60 34.732 60 35.963	68.976 69.499 69.890 70.417	-9.169 1.00 -7.177 1.00 -9.882 1.00 -7.877 1.00 -9.234 1.00	206.05 206.05 206.05 206.05
3517 CZ 3518 C 3519 O	PHE B	60 35.732 60 33.073 60 32.479 61 32.911	70.612 66.407 66.957 65.125	-4.968 1.00 -4.044 1.00 -5.257 1.00 -4.520 1.00	146.51 146.51 158.05 158.05
3521 CA 3522 CB 3523 CG	GLU B GLU B GLU B GLU B	61 31.977 61 31.872 61 31.394 61 32.288	64.284 62.911 62.950 63.798	-5.197 1.00 -6.651 1.00 -7.556 1.00 -7.574 1.00	249.69 249.69 249.69 249.69
3524 CD 30 3525 OE1 3526 OE2 3527 C 3528 O	GLU B GLU B GLU B GLU B	61 33.522 61 31.753 61 32.391 61 31.555	63.580 64.685 64.113 63.831 64.285	-8.256 1.00 -3.067 1.00 -2.213 1.00 -2.789 1.00	249.69 158.05 158.05 134.92
3529 N 3529 N 35 3530 CA 3531 CB 3532 CG	ASP B ASP B ASP B ASP B	62 33.682 62 34.200 62 35.729 62 36.294	64.139 64.128 63.118 62.048	-1.426 1.00 -1.432 1.00 -2.393 1.00 -2.551 1.00	134.92 133.92 133.92 133.92
3533 OD1 3534 OD2 40 3535 C 3536 O	ASP B ASP B ASP B ASP B	62 35.669 62 37.364 62 33.709 62 33.663 63 33.358	63.397 65.279 65.143 66.400	-2.972 1.00 -0.543 1.00 0.685 1.00 -1.177 1.00	133.92 134.92 134.92 128.21
3537 N 3538 CA 3539 CB 45 3540 OG	SER B SER B SER B	63 32.857 63 32.552 63 33.696	67.553 68.710 69.095 67.137	-0.449 1.00 -1.407 1.00 -2.153 1.00 0.261 1.00	212.43 128.21
3541 C 3542 O 3543 N 3544 CA	SER B SER B GLY B GLY B	63 30.660 64 31.500 64 30.298	66.629 67.347 66.963 66.973	-0.377 1.00 1.571 1.00 2.274 1.00 3.784 1.00	137.99 137.99 137.99
50 3545 C 3546 O 3547 N 3548 CA	GLY B GLU B GLU B	64 30.367 64 31.282 65 29.378 65 29.219 65 27.747	67.545 66.312 66.217 66.504	4,385 1.00 4,383 1.00 5,830 1.00 6,159 1.00	125.38 0 125.38 0 249.57
3549 CB 55 3550 CG 3551 CD 3552 QE1		65 27.329 65 25.818 65 25.227 65 25.217	66.290 66.198 65.270 67.046	7.594 1.0 7.731 1.0 7.143 1.0 8.416 1.0 6.339 1.0	0 249.57 0 249.57 0 249.57
3553 OE2 3554 C 60 3555 O 3556 N	GLU B GLU B TYR B TYR B	65 29.617 65 29.050 66 30.575 66 31.029	64.843 63.844 64.790 63.510	5.900 1.0 7.265 1.0 7.826 1.0	00 125.38 00 138.71 00 138.71
3557 CA 3558 CB 3559 CQ 65 3560 CD	TYR B TYR B 1 TYR B	66 32.512 66 32.917 66 32.997 66 33.473	63.294 63.170 64.287 64.189	6.122 1.5 5.302 1.3.998 1.	00 186.43 00 186.43 00 186.43 00 186.43
3561 CE 3562 CD 3563 CE 3564 CZ 70 3565 OH	2 TYR B 2 TYR B TYR B	66 33.309 66 33.785 66 33.871 66 34.375	61.943 61.827 62.957 . 62.850	4.314 1. 3.508 1	.00 186.43 .00 186.43 .00 186.43

					00.002	63.378	9.345	1.00	138.71
	3566	С		66	30.823 30.510	64.370	10.022	1.00	138.71
	3567	0	–	66	31.029	62.155	9.862	1.00	179.70
	3568	N		67 67	30.895	61.847	11.295	1.00	179.70 159.69
	3569	CA	LYS B	67	29.456	62.047	11.754	1.00	159.69
5	3570	CB	LYS B	67	28.447	61.317	10.919 11.392	1.00 1.00	159.69
	3571	CD CD	LYS B	67	27.057	61.654	10.324	1.00	159.69
	3572	CE	LYS B	67	26.005	61.334	10.773	1.00	159.69
	3573 3574	NZ	LYS B	67	24.591	61.613 60.434	11.691	1.00	179.70
10	3575	Ċ	LYS B	67	31.323	59.505	10.885	1.00	179.70
10	3576	0	LYS B	67	31.284 31.723	60.285	12.953	1.00	162.03
	3577	N	CYS B	68 68	32.142	58.993	13.489	1.00	162.03 162.03
	3578	ÇA	CYS B	68	31.445	58.691	14.810	1.00 1.00	162.03
	3579	C	CYS B	68	31.102	59.589	15.578 13.665	1.00	220.63
15	3580	O CB	CYS B	68	33.670	58.915	14.951	1.00	220.63
	3581	SG	CYS B	68	34.426	59.969 57.402	15.049	1.00	249.69
	3582 3583	N	GLN B	69	31.239	56.906	16.245	1.00	249.69
	3584	CA	GLN B	69	30.573 29.078	56.763	15. 965	1.00	222.67
20	3585	СВ	GLN B	69 69	28.343	55.832	16. 904	1.00	222.67 222.67
	3586	ca	GLN B GLN B	69	26.898	55.619	16.496	1.00 1.00	222.67
	3587	CD	GLN B	69	26.612	55.268	15.351 17.435	1.00	222.67
	3588	OE1 NE2	GLN B	69	25.977	55.823	16.606	1.00	249.69
05	3589	C	GLN B	69	31.168	55.546	15.727	1.00	249.69
25	3590 3591	ŏ	GLN B	69	31.580	54.788 55.235	17.897	1.00	249.63
	3592	Ň	HIS B	70	31.219	53.956	18.331	1.00	249.63
	3593	CA	HIS B	70 70	31.762 32.637	54.139	19.570	1.00	248.69
	3594	CB	HIS B	70 70	33.932	54.841	19.289	1.00	248.69 248.69
30	3595	CG	HIS B HIS B	70	34,500	55.925	19.864	1.00 1.00	248.69
	3596	CD2 ND1	HIS B	70	34.798	54.422	18.304 18.283	1.00	248.69
	3597	CE1	HIS B	70	35.852	55.223 56.141	19.217	1.00	248.69
	3598 3599	NE2	HIS B	70	35.696	52.952	18.618	1.00	249.63
35	3600	C	HIS B	70	30.656 29.488	53.196	18.308	1.00	249.63
55	3601	0	HIS B	70 71	31.032	51.824	19.211	1.00	249.69 249.69
	3602	N	GLN B	71	30.087	50.755	19.541	1.00 1.00	249.69
	3603	CA	GLN B	71	30.836	49.613	20,251 20,254	1.00	249.69
40	3604	CB CG	GLN B	71	30.136	48.247	18.850	1.00	249.69
40	3605 3606	CD	GLN B	71	29.921	47.672 47.657	18.016	1.00	249.69
	3607	OE1	GLN B	71	30.834 28.710	47.183	18.594	1.00	249.69
	3608	NE2	GLN B	71	28.923	51.253	20.410	1.00	249.69 249.69
	3609	C	GLN B GLN B	71 71		50.990	20.118	1.00 1.00	249.69
45		0	GLN B GLN B	72		51.983	21.471 22.371	1.00	249.69
	3611	N CA	GLN B	72	28.217	52.506	23.671	1.00	249.69
	3612	CB	GLN B	72		51.678 52.118	24.772	4 00	249.69
	3613 3614	ČĠ	GLN B	72		51.390	26.084	1.00	249.69
50	3615	CD	GLN B	72		50.159	26.130		249.69
<u> </u>	3616	OE1	GLN B	7: 7:		52.151	27.156		249.69 249.69
	3617	NE2	GLN B GLN B			53.997	22.656		249.69
	3618	C	GLN B	_	2 28.598	54.423	23.809 21.588		249.69
_	3619	0 N	VAL B		3 28.533	54.787	21.71		249.69
5	5 3620 3621	CA	VAL E	3 7	3 28.747	56.226 56.626	21.45	g 1.00	227.88
	3622	CB	VAL E		3 30.224		21.91	7 1.00	227.88
	3623	CG1	VAL E		r3 30.454 r3 31.167		22.17		227.88 249.69
	3624	CG2	VAL E		r3 31.167 73 27.875		20.69		249.69
6	50 3625	Ç	VAL E		73 27.681	56.449	19.57		249.69
	3626	0	ASN I	-	74 27.348	58.101	21.06 20.15		249.69
	3627	N CA	ASN	-	74 26.504		20.15		218.87
	3628 3629	CB	ASN	В	74 25.675	40.007	22.0		218.87
	65 3630	čā	ASN	В	74 24.852		21.84	45 1.00	218.87
,	3631	OD1			74 24.270 74 24.793		23.2		218.87 249.69
	3632	ND2	ASN	_	74 24.79 74 27.36		19.1		
	3633	C	ASN ASN	В	74 28.34	2 60.240	19.4		
	3634	0	GLU		75 27.00	5 59.383	17.8		
	70 3635	.,			,				

							16.704	1.00	242.43
		CA	GLU B	75 [*]	27.735	59.968		1.00	240.14
	3636				26.889	59.853	15.429		
	3637	CB			25.394	60.044	15.649	1.00	240.14
	3638	CG	GLU B	75		59.681	14,423	1,00	240.14
		CD	GLU B	75	24.571		13.867	1.00	240.14
_	3639	OE1	GLU B	7 5	24.782	58.580			240.14
5	3640		GLU B	75	23.709	60.493	14.021	1.00	
	3641	OE2				61.410	16.900	1.00	242.43
	3642	С	GLU B	75	28.199	62.241	17.453	1.00	242.43
		Ŏ	GLU B	75	27.478		16.427	1.00	249.69
	3643		SER B	76	29.413	61.690			
	3644	N		76	30.030	63.012	16.552	1.00	249.69
10	3645	CA	SER B			62.960	16.091	1.00	193.15
	3646	CB	SER B	76	31.491		14.681	1.00	193.15
		OG	SER B	76	31.574	62.865		1.00	249.69
	3647		SER B	76	29.323	64.104	15.766		249.69
	3648	Ç		76	28.595	63.825	14.813	1.00	
	3649	0	SER B			65.351	16.175	1.00	227.37
15	3650	N	GLU B	77	29.555	00.001	15.500	1.00	227.37
IJ		CA	GLU B	77	28.969	66.496		1.00	249.69
	3651		GLU B	77	29.300	67.790	16.252		249.69
	3652	CB		77	28.667	67.874	17.635	1.00	
	3653	CG	GLU B			67.885	17.588	1.00	249.69
	3654	CD	GLU B	77	27.144		16.493	1.00	249.69
20		OE1	GLU B	77	26.566	67.679		1.00	249.69
20	3655		GLU B	77	26.521	68.094	18.654		227.37
	3656	OE2		77	29.556	66.554	14.099	1.00	
	3657	С	GLU B			66.802	13.926	1.00	227.37
	3658	0	GLU B	77	30.747		13.072	1.00	151.66 ·
		Ň	PRO B	78	28.708	66.324		1.00	139.99
~~	3659		PRO B	78	27.233	66.271	13.163		151.66
25	3660	CD	7000	78	29.168	66.339	11.671	1.00	
	3661	CA	PRO B		27.852	66.486	10.892	1.00	139.99
	3662	CB	PRO B	78		65.808	11.784	1.00	139.99
		CG	PRO B	78	26.833			1,00	151.66
	3663	_	PRO B	78	30.136	67.473	11.369		151.66
	3664	Ç		78	30,182	68.466	12.086	1.00	
30	3665	0	PRO B		30.929	67.306	10.321	1.00	174.84
	3666	N	VAL B	79		68.352	9,905	1.00	174.84
	3667	CA	VAL B	79	31.855		10.222	1.00	152.46
		СВ	VAL B	79	33. 33 6	68.021			152.46
	3668		VAL B	79	34.256	69.029	9.536	1.00	
	3669	CG1			33.566	68.076	11.714	1.00	152.46
35	3670	CG2	VAL B	79		68.435	8.405	1.00	174.84
JJ	3671	C	VAL B	79	31.682		7.752	1.00	174.84
		ŏ	VAL B	79	31.482	67.408		1.00	124.58
	3672		TYR B	80	31.738	69.642	7.850		124.58
	3673	N		80	31.564	69.771	6.414	1.00	
	3674	CA	TYR B			70.877	6.084	1.00	201.47
40	3675	CB	TYR B	80	30.573		4.675	1.00	201.47
70		CG	TYR B	80	30.044	70.777		1.00	201.47
	3676		TYR B	80	28.979	69.936	4.370		201.47
	3677	CD1		80	28.515	69.801	3.072	1.00	
	3678	CE1	TYR B		30.636	71.484	3.641	1.00	201.47
	3679	CD2	TYR B	80			2,334	1.00	201.47
45	3680	CE2	TYR B	80	30.180	71.356	2.057	1.00	201.47
4,5		CZ	TYR B	80	29.122	70.514			201.47
	3681			BO	28.676	70.383	0.762	1.00	
	3682	OH			32.861	70.049	5.704	1.00	124.58
	3683	С	TYR B	80		70.887	6.140	1.00	124.58
	3684	0	TYR B	80			4.606	1.00	114.91
	3004	Ň	LEU B	81	33.082	69.344			114.91
50			LEU B	81	34.296	69.544	3.839	1.00	
	3686	CA				68.223	3.661	1.00	104.59
	3687	CB	LEU B	81		68.327	2,720	1.00	104.59
	3688	CG	LEU B	81	36.234		3.327	1.00	104.59
		CD1	LEU B	81	37.234	69.306			104.59
	_ 3689		LFII B	81		66.972	2.487		
5:	5 3890	CD2				70.087	2,482	1.00	114.91
	3691	С	LEU B	81		69.517	1.836	1.00	114.91
	3692	0	LEU B	81			2.049		120.70
		Ň	GLU B	82	2 34.545	71.184			120.70
	3693		GLU B	82		71.734	0.72		201.66
	3694	CA				73.163	0.83		
6	0 3695	СВ	GLU B			73.551	-0.33	2 1.00	201.66
•	3696	CG	GLU B	. 8:	2 32.820	70.001	-0.21		201.66
		CD	GLU B	8	2 32.280	74.954			201.66
	3697		GLU B	Ā	2 32.022	75.401	0.92		201.66
	3698	OE1		_	2 32.100	75.610	-1.26		
	3699	OE2	GLU B	_			-0.17	4 1.00	120.70
6	5 3700	С	GLU B		2 35.482		0.27		120.70
·	3701	ō	GLU E	3 8	2 36.583		-1.43		157.10
		Ň	VAL E		35.299	71.276			157.10
	3702		VAL E	-	33 36.398		-2,39		
	3703	CA				69.829	-3.03		142.28
	3704	СВ	VAL E				-4.00	5 1.00	142.28
-	70 3705	CG1	VAL E	3 (83 37.69 9	09.020			
	, , , ,,,,,								

						68.770	-1.955	1.00	142.28
	3706	CG2	****	B3 ⁻	36.708	72.239	-3.494	1.00	157.10
	3707	C	*/10 -	83	36.227 35.120	72.455	-3.992	1.00	157.10
	3708	0		83 84	37.344	72.845	-3.895	1.00	122.91 122.91
	3709	N	PHE B	84	37.331	73.921	-4.875	1.00 1.00	156.44
	3710	CA	PHE B PHE B	84	37.654	75.240	-4.180 -3.106	1.00	156.44
	3711	CB CG	PHE B	84	36.687	75.629	-1.821	1.00	156.44
	3712	CD1	PHE B	84	36.773	75.093 76.562	-3.382	1.00	156.44
	3713 3714	CD2	PHE B	84	35.696	75.485	-0.833	1.00	156.44
10	3715	CE1	PHE B	84	35.885 34.805	76.958	-2.401	1.00	156.44
10	3716	CE2	PHE B	84 84	34.903	76.419	-1.121	1.00 1.00	156.44 122.91
	3717	CZ	PHE B PHE B	84	38.259	73.854	-6.045 6.007	1.00	122.91
	3718	C	PHE B	84	39.300	73.198	-6.007 -7.064	1.00	152.63
	3719	0 N	SER B	85	37.884	74.614 74.765	-8.267	1.00	152.63
15	3720 3721	CA	SER B	85	38.690	74.080	-9.467	1.00	143.15
	3722	CB	SER B	85	38.054 38.872	74.255	-10.617	1.00	143.15
	3723	OG	SER B	85 85	38.741	76.262	-8.523	1.00	152.63 152.63
	3724	Ç	SER B SER B	85	37.715	76.882	-8.796	1.00 1.00	139.36
20	3725	0	ASP B	86	39.933	76.836	-8.412 -8.613	1.00	139.36
	3726	N CA	ASP B	86	40.120	78.263	-8.613 -7.577	1.00	172.94
	3727	CB	ASP B	86	39.314	79.047 80.313	-8.143	1.00	172.94
	3728 3729	CG	ASP B	86	38.724	81.114	-8.744	1.00	172.94
25	3730	OD1	ASP B	86	39.476 37.505	80.511	-7.977	1.00	172.94
23	3731	OD2	ASP B	86 86	41.606	78.609	-8.458	1.00	139.36 139.36
	3732	C	ASP B	86	42.379	77.794	-7.963	1.00 1.00	121.62
	3733	0	ASP B TRP B	87	42.003	79.814	-8.863 -8.745	1.00	121.62
	3734	N CA	TRP B	87	43.393	80.224	-9.459	1.00	247.13
. 30	3735	CB	TRP B	87	43.617	81.544 81.344	-10.891	1.00	247.13
	3736 3737	CG	TRP B	87	43.989	81.328	-12.013	1.00	247.13
	3738	CD2	TRP B	87	43.103 43.881	81.063	-13.164	1.00	247.13 247.13
	3739	CE2	TRP B TRP B	87 87		81.521	-12.166	1,00 1.00	247.13
35	3740	CE3	TRP B	87	45.237	81.085	-11.386 -12.752	1.00	247.13
	3741	CD1 NE1	TRP B	87		80.918	-14.445	1.00	247.13
	3742	CZ2	TRP B	87		80.982 81.442	-13.443	1.00	247.13
	3743 3744	CZ3	TRP B	87		81.171	-14.563	1.00	247.13
40		CH2	TRP B	87		80.336	-7.288	1.00	121.62 121.62
40	3746	С	TRP B	87 87	·	79.726	-6.870		133.11
	3747	0	TRP B	8		81.106	-6.510 -5.092		133.11
	3748	N	LEU B	8	8 43.333	81.246	-5.0 5 2 -4.789		136.45
4.4	3749	CA CB	LEU B	8		82.678 83.123	-5.444		130.45
45	3750 3751	čG	LEU B		8 45.105	84.525	-4.973	3 1.00	136.45
	3752	CD1	LEU B		8 45.489 8 46.196	82.131	-5.093		136.45 133.11
	3753	CD2	LEU B		18 46.196 18 42.137	80.876	-4.219		133.11
	3754	C	LEU B LEU B		8 40.985	81.159	-4.57 -3.08	•	126.96
5	0 3755	0	LEU B		89 42.413	80.222	-3.06 -2.14		126.96
	3756	N GA	LEU B		89 41.363	79.834 78.335	-2.15		168.49
	3757 3758	CB	LEV B	1 1	89 41.152	77.8 6 5	-1.13	1.00	166.49
	3759	CG	LEU E		89 40.113 89 38.812	040	-1.30	6 1.00	156.49 (38.49
5	5 3760	CD1	LEU E		89 38.812 89 39.881		-1.30		126.96
_	3761	CD2	LEU E		89 41.777	80.255	-0.74		126.96
	3762	C	LEU I	-	89 42.900	79.978	-0.33 -0.03		113.68
	3763	0 N	LEU		90 40.883		1.3		113.68
	3764	CA	LEU		90 41.196		1.6	46 1.00	125.93
,	60 3765 3766	CB	LEU		90 40.422 90 40.530		3.1		125.93 125.93
	3767	CG	LEU	В	90 40.534 90 41.98		3.4		125.93
	3768	CD1		8	90 39.69		3.3		
	3769	CD	LEU	8	90 40.85	6 80.326		356 1.00 566 1.00	
	65 3770	CO	LEU	B	90 39.69	3 80.010		010 1.00	98.97
	3771		GLN	В	91 41.87			000 1.00	98.97
	3772 3773		GLN	В	91 41.64			842 1.00	
	3774	СВ	GLN		91 42.66 91 42.65		2.	481 1.00	171.07
	70 3775		GLN	В	91 42.65				

							2,363	1.00	171.07
		CD	GLN B	91 [.]	43.685	75.865	2.555 2.555	1.00	171.07
	3776	OE1		91	44.878	76.095 74.660	2.046	1.00	171.07
	3777	NE2	GLN B	91	43.232	74.660 79.237	5.422	1.00	98.97
	3778 3779	Ċ.		91	41.707	80.023	5.780	1.00	98.97
5	3780	0		91	42.592 40.769	78.773	6.244	1.00	123.57
	3781	N	,	92 92	40.707	79.189	7.645	1.00	123.57 155.46
	3782	CA	ALA B ALA B	92	39.422	79.967	7.914	1.00 1.00	123.57
	3783	СВ	ALA B	92	40.774	77.974	8.537 8.208	1.00	123.57
4.0	3784	C O	ALA B	92	40.215	76.918	9.662	1.00	119.49
10	3785	N	SER B	93	41.473	78.126 77.046	10.652	1.00	119.49
	3786	CA	SER B	93	41.631	77.561	11.897	1.00	144.43
	3787 3788	CB	SER B	93	42.377 41.794	78.730	12.443	1.00	144.43
	3789	OG	SER B	93	41.794	76.547	11.026	1.00	119.49
15	3790	С	SER B	93 93	39.891	75.389	10.783	1.00	119.49 139.25
	3791	0	SER B ALA B	94	39.447	77.448	11.605	1.00 1.00	139.25
	3792	N CA	ALA B	94	38.072	77.173	11.989 13.497	1.00	173.88
	3793	GA ⊕B	ALA B	94	37.961	77.053	11.484	1.00	139.25
20	3794	Č	ALA B	94	37.289	78.378 79.465	11.346	1.00	139.25
20	3795 3796	ŏ	ALA B	94	37.843	78.197	11.188	1.00	153.31
	3797	N	GLU B	95	36.010 35.217	79.312	10.694	1.00	153.31
	3798	CA	GLU B	95 95	34.219	78.813	9.648	1.00	193.17 193.17
	3799	CB	GLU B GLU B	95 95	34.894	78.235	8.419	1.00 1.00	193.17
25	3800	cG	GLU B	95	33.929	77.974	7.284	1.00	193.17
	3801	CD QE1	GLU B	95	34.372	77.478	6. 23 0 7.442	1.00	193.17
	3802	OE2	GLU B	95	32.727	78.269 80.058	11.817	1.00	153.31
	3803 3804	C	GLU B	95	34.493	81.241	11.678	1.00	153.31
30	3804	ŏ	GLU B	95	34.153	79.364	12.930	1.00	119.30
30	3806	N	VAL B	96	34.272 33.599	79.942	14.087	1.00	119.30 135.82
	3807	CA	VAL B	96 96	32.262	79.239	14.355	1.00	135.82
	3808	CB	VAL B VAL B	96	31.387	80.129	15.250	1.00 1.00	135.82
	3809	CG1	VAL B	96	31.566	78.905	13.045 15.330	1.00	119.30
35	3810	CG2 C	VAL B	96	34.482	79.788	15.622	1.00	119.30
	3811	ŏ	VAL B	96	34.967	78.690 80.871	16.082	1.00	139.44
	3812 3813	Ň	VAL B	97	34.664 35.530	80.799	17.247	1.00	139.44
	3814	CA	VAL B	97	36.882	81.401	16.927	1.00	116.73 116.73
40	3815	СВ	VAL B	97 97		80.880	17.910		116.73
	3816	CG1	VAL B VAL B	97		81.074	15.506		139.44
	3817	CG2	VAL B	97	35.070	81.451	18.543 18.528		139.44
	3818	C O	VAL B	97		8 <u>2.445</u> 80.882	19.659		148.58
45	3819 3820	Ň	MET B	98		80.862 81.363	21.015	5 1.00	148.58
4.	3821	CA	MET B	98		80.224	22.03	4 1.00	249.69
	3822	СВ	MET B	91		79.059	21.89		249.69 249.69
	3823	ÇG	MET B	9		79.444	22.53		249.69
_	3824	SD CE	MET B MET B	9	8 33.078	79.331	24.29 21.36		148.58
5	0 3825	C	MET B		8 36.217	82.467	21.30		148.58
	3826	ŏ	MET B	9	8 37.425		21.75		152.43
	3827 3828	Ň	GLU B	. 9	9 35.721	- 4 75 4	22.10	1.60	152.43
	3829	CA	GLU B		9 38.604 19 35.865	A	22.97		244.45 244.45
5	5 3830	CL	GLU B		99 35.865 99 36.447		22.89		244.45
	3831	CG	GLU E		99 35.89	88.095	23.95 24.20		244.45
	3832	CD		-	99 34.68	87.989	24.4		244.45
	3833	OE1 OE2			99 36.66	-4004	22.8		152.43
	3834 5() 3835	Č	GLU (В	99 37.83		23.8	77 1.00	152.43
,	5O 3835 3836	ŏ	GLU.	_	99 37.70	04 506	22.3	63 1.00	146.37
	3837	N	GLY		100 39.01 100 40.21		23.0		146.37 146.37
	3838	ÇA	GLY		100 40.21 100 41.00	6 83.025	22.3		440.07
	3839	C	GLY GLY	B	100 42.20	ys 82.880	22.0		400.40
	65 3840	0	GLY	B	101 40.3	₅₃ 82.237	21.5 20.5		400.40
	. 3841	N CA	GLN	В	101 41.00			290 1.00	190.16
	3842 3843		GLN	В	101 39.9			346 1.00	190.16
	3844	CG	GLN	В	101 39.2 101 40.2			370 1.00	190.16
	70 3845		GLN	B	101 40.2				

	B46 847	OE1 NE2	GLN B	101 101	40.792 40.441 41.952	79.645 77.565 81.596	23.140 22.378 19.731	1.00 1.00 1.00	190.16 190.16 128.49
	848	C	GLN B	101 101	42.038	82.780	19.407	1.00 1.00	128.49 164.10
.3	849	0	GLN B PRO B	102	42.675	80.637	19.115 19.540	1.00	192.64
	1850	N CD	PRO B	102	42.886	79,258 81,010	18.018	1.00	164.10
	1851 3852	CA	PRO B	102	43.581	79.950	18.152	1.00	192.64
	3853	CB	PRO B	102 102	44.669 43.863	78.733	18.490	1.00 1.00	192.64 164.10
	3854	CG	PRO B PRO B	102	42.928	80.983	16.652 16.389	1.00	164.10
	3855	CO	PRO B	102	42.017	80.208 81.831	15.761	1.00	147.70
	3856 2057	N	LEU B	103	43.418	81.913	14.425	1.00	147.70
	3857 3858	CA	LEU B	103	42.870 41.981	83.136	14.328	1.00	111.28 111.28
	3859	CB	LEU B	103 103	41.244	83.102	13.004	1.00 1.00	111.28
15	3860	CG	LEU B LEU B	103	40.261	81.951	13.100 12.716	1.00	111.28
	3861	CD1 CD2	LEU B	103	40.546	84.415 81.997	13.331	1.00	147.70
	3862 3863	C	LEU B	103	43.939 44.797	82.868	13.379	1.00	147.70 122.26
	3864	Ō	LEU B	103 104	43.890	81.112	12.339	1.00	122.26
20	3865	N	PHE B PHE B	104	44.880	81.157	11.261 11.311	1.00 1.00	249.69
	3866	CA CB	PHE B	104	45.820	79.951	12.627	1.00	249.69
	3867	CG	PHE B	104	46.501	79.766 79.216	13.707	1.00	249.69
	3868 3869	CD1	PHE B	104	45.816 47.831	80.137	12.793	1.00	249.69 249.69
25	3870	CD2	PHE B	104 104		79.041	14.939	1.00 1.00	249.69
	3871	CE1	PHE B PHE B	104		79.967	14.020 15.096	1.00	249.69
	3872	CE2 CZ	PHE B	104	47.773	79.416 81.185	9.885	1.00	122.26
	3873 3874	Č	PHE B	104		80.290	9.546	1.00	122.26
30	3875	Ö	PHE B	104 109		82.207	9.093		122.11 122.11
50	3876	N	LEU B LEU B	10		82.309	7.743 7.495		103.82
	3877	CA	LEU B	10	5 43.39 0	83.676	7.493 8.466		103.82
	3878	CB CB	LEU B	10		, 84.000 85.309	8.040	1.00	103.82
35	3879 3880	CD1	LEU B	10		82.847	8.512		103.82 122.11
33	3881	CD2	LEU B	10 10		82.083	6.776		122.11
	3882	C	LEU B	10	5 46.272	82.387	7.065 5.600		131.12
	3883	O N	ARG B	10		81.560 81.289	4.64	5 1.00	131.12
40	3884 3885	CA	ARG B		06 45.870 06 46.287		4.79	2 1.00	175.38 175.38
40	3886	CB	ARG B		06 46.287 06 47.38		3.87		175.38
	3887	ca	ARG B		06 47.59	3 77.897	3.98 2.97		175.38
	3888	CD NE	ARG B		06 48.54		2.40	1.00	175.38
45	3889 3890	CZ	ARG B		06 48.53 06 47.61		2.74	13 1.00	175.38 175.38
45	3891	NH1	ARG B		06 47.61 106 49.43		1.47	77 1.00 20 1.00	131.12
	3892	NH2	ARG B		06 45.41	81.578	3.2 2.7	:	131.12
	3893	C	ARG		106 44.37		2.5	07 1.00	139.30
50	3894) 3895	N	CYS E	3	107 46.10		1.1	24 1.00	139.30 139.30
3(3896	SA	CYS		107 45.8 107 46.5	04.564	0.3		139.30
	3897	C	CYS I		107 47.7	47 81.560		598 1.00	152.04
	3898	O CB	CYS	В	107 46.4		^ ^	1.00	152.04
5	3899 5 3900	SG	CYS	В	107 45.8			073 1.00	155.54 155.54
3	3901	N		В	108 45.7 108 46.2	446	, -0.7	771 1.00	137.70
	3902	CA		B B∙	108 45.4	129 78.18 0		319 1.00 745 1.00	
	3903	CB	HIS	В	108 46.0	047 76.88 ⁰		357 1.00	137.70
	3904	. CG CD2		В	108 45.			486 1.00	
•	50 3905 3906	ND1	I HIS	В		366 76.56 609 75.34	1 -0.	.919 1.00	
	3907	CE1	I HIS	В		506 74.85	4 -1	.453 1.00 289 1.00	
	3908		2 HIS	B B		.182 79.48	" ^	.289 1.00 .900 1.00	155.54
	3909		HIS	В	108 45	137 79.73 351 79.25	"	881 1.0	164.07
	65 3910 3911		GLY	В			~ 71 -4	1.321 1.0	
	3912	CA	GLY	8		.090 77.9	15	1.866 1.0 1.098 1.0	104.07
	3913	3 <u>C</u>	GLY GLY	В		.967 76.9	70	4.098 1.0 6.180 1.0	
	3914		TRP	В		5.886 . 77.8°	33 °	v. 100	
	70 391	9 1			•				

							0.040	1.00	153.07
		ĊA	TRP B	110 46.5		76.568	-6.812 -8.097	1.00	171.40
	3916	CB		110 45.7	719 7	76.839	-8.920	1.00	171,40
	3917	CG		110 45.4		75.611	-8.973	1.00	171.40
	3918	CD2		110 44.2		74.833 73.764	-9.855	1.00	171.40
5	3919 3920	CE2	TRP B	110 44.4	,,,,	74.937	-8.353	1.00	171.40
,	3921	CE3		110 42.5	500	75.000	-9.745	1.00	171.40
	3922	CD1	,,,,,	110 46.		73.889	-10.311	1.00	171.40
	3923	NE1	TRP B			72.799	-10.140	1.00	171.40
	3924	CZ2	TRP B TRP B		026	73.974	-8.639	1.00	171.40 171.40
10	3925	CZ3	TRP B TRP B		297	72.921	-9.526	1.00 1.00	153.07
	3926	CH2	TRP B		743	75.723	-7.098 -7.296	1.00	153.07
	3927	C O	TRP B	110 48.	.833	76.257	-7.2 9 0 -7.104	1.00	188.19
	3928	N	ARG B		.567	74.404 73.481	-7.333	1.00	188.19
15	3929 3930	CA	ARG B	• • • •	.671	73.522	-8.790	1.00	249.69
13	3931	СВ	ARG B		.124	72.532	-9.682	1.00	249.69
	3932	CG	ARG B	* * * *	.394 .101	72.359	-11.018	1.00	249.69
	3933	CD	ARG B		.005	70.961	-11.448	1.00	249.69 249.69
	3934	NE	ARG B ARG B		.641	69.965	-10.751	1.00 1.00	249.69
20	3935	CZ	ARG B).241	70.210	-9.587	1.00	249.69
	3936	NH1 NH2	ARG B	111 49	9.594	68.722	-11.216 -6.431	1.00	188.19
	3937 3938	C	ARG B		9.845	73.814	-6.787	1.00	188.19
	3939	ŏ	ARG B	• • • -	0.999	73.588 74.350	-5.260	1.00	160.66
25	3940	Ň	ASN B		9.534	74.330 74.729	-4.291	1.00	160.66
23	3941	CA	ASN B		0.542 1.146	73.478	-3,648	1.00	209.47
	3942	CB	ASN B		1.910	73.791	-2.372	1.00	209.47 209.47
	3943	CG	ASN B	112 5	2.226	74.94 7	-2.083	1.00	209.47
	3944	OD1	ASN B ASN B		2.221	72.757	-1.607	1.00 1.00	160.66
30	3945	ND2	ASN B		1.652	75.583	-4.931 -4.489	1.00	160.66
	3946	C	ASN B		2.808	75.522	-5.966	1.00	180.98
	3947 3948	Ň	TRP B		1.319	76.368 77.223	-6.608	1.00	180.98
	3949	CA	TRP B		52.321	77.888	-7.863	1.00	248.40
35		CB	TRP B	*	51.781 51.824	77.037	-9.064	1.00	248.40
-	3951	CG	TRP B		50.876	77.029	-10.131	1.00	248.40 248.40
	3952	CD2	TRP B TRP B		51.344	76.102	-11.092	1.00 1.00	248.40
	3953	CE2 CE3	TRP B		49.678	77.717	-10.370	1.00	248.40
40	3954	CD1	TRP B	113	52.799	76.145	-9,405 -10.623	1.00	248.40
40) 3955 3956	NE1	TRP B		52.513	75.582 75.845	-12.289	1.00	248.40
	3957	CZ2	TRP B	,	50.639	75.845 77.461	-11.557	1.00	248.40
	3958	CZ3	TRP B		48.984 49. 47 2	76.530	-12.504	1.00	248.40
	3959	CH2	TRP B	113 113	52.741	78.311	-5.641	1.00	180.98 180.98
4:		Ç	TRP B	113	52.414	78.261	-4.452	1.00 1.00	240.61
	3961	0 N	ASP B	114	53.465	79.305	-6.144 -5. 29 2	1.00	240.61
	3962	CA	ASP B	114	53.905	80.407	-5.292 -5.390	1.00	249.69
	3 963 3964	CB	ASP B	114	55.427	80.596 79.633	-4.489	1.00	249.69
5	0 3965	CG	ASP B	114	56.207	79.644	-3.260	1.00	249.69
,	3966	OD1	ASP B	114	55.981 57.054	78.868	-5.007	1.00	249.69
	3967	OD2	ASP B	114 114	53.185	81.707	-5.655		240.61 240.61
	3968	C	ASP B ASP B	114	53.064	82.062	-6.841		153.55
	3969	0	VAL B		52.691	82.403	-4.627 -4.828		153.55
:	5 3970	N CA	VAL B		51.976	83.665	-4.820 -4.135		146.14
	3971 3972	CB	VAL B	115	50.603	83.666 84.824	-4.640		146.14
	3973	CG1	VAL B		49.770	82.359	-4.38		146.14
	3974	CG2	VAL B		49.887 52.790	84.823	-4.25		153.55 153.55
(60 3975	С	VAL B		53.410	84.708	-3.19		165.97
	3976	0	VAL B		52.781	85.939	-4.97		165.97
	3977	N	TYR B		53.518	87.128	-4.57 -5.61		249.69
	3978	CA CB	TYR E		54.595	87.441	-5.72		249.69
	3979 65 3980	CG	TYR E	3 116	55.660	86.371 85.393	-5.72 -6.71		249.69
	3981	CD1	TYR	B 116	55.612	84.386	-6.78	1.00	249.69
	3982	CE1	TYR		56.582 56.700	86.319	-4.80	1.00	249.69
	3983	CD2				85.322	-4.85		249.69 249.69
	3984	CE2	2 TYR I TYR I	<u>-</u>		84.360	-5.84	1.00	<u> </u>
	70 3985	cz	LIP I			•			

	3986 3987 3988	CO	TYR B TYR B TYR B LYS B	116 116 116 117	58.575 52.593 51.423 53.129	88 88 89	.375 .332 .278	-5.898 -4.405 -4.782 -3.840 -3.609	1.00 1.00 1.00 1.00 1.00	249.69 165.97 165.97 123.89 123.89
5	3989 3990 3991 3992	N CA CB CG	LYS B LYS B LYS B	117 117 117	52.369 52.154 53.310 52.850	91 92	1.641 1.413 2.323 3.384	-4.924 -5.333 -6.340	1.00 1.00 1.00 1.00	248.40 248.40 248.40 248.40
	3993 3994	CD CE	LYS B	117	51.729 51.232	94	4.253 5.311	-5.761 -6.687	1.00 1.00	248.40 123.89
10	3995	NZ C	LYS B LYS B	117	51.019 49.97	9	0.378 0.844	-2.948 -3.409	1.00	123.89 126.95
	3996 3997	O N	LYS B VAL B	117	51.05	5 8	9.650 19.314	-1.846 -1.142	1.00	126.95 114.58
	3998 3999	CA CB	VAL B VAL B	118 118	49.84 50.03	3	37.999 37.892	-0.408 0.760	1.00	114.58 114.58
15	4000 4001	CG1 CG2	VAL B VAL B	118 118	49.07 49.78	19	86.867 90.352	-1.372 -0.177	1.00 1.00	126.95
	4002 4003	С	VAL B	118 118	50.05	51	91.007	0.547 -0.179	1.00 1.00	126.95 120.13
20	4004 4005	O N	ILE B	119 119	47.9	44	90.477 91.402	0.686 -0.073	1.00 1.00	120.13 113.05
20	4006 4007	CA CB	ILE B	119	46.8	.0	92.633 93.628	0.860	1.00 1.00	113.05 113.05
	4008 4009	CG2 CG1	ILE B ILE B	119	9 48.0	21	93.233 94.049	-0.750 -1.930	1.00	113.05 120.13
25	4010	CD1 C	ILE B	119	9 45.9	71	90.716 90.135	1.152 0.347	1.00 1.00	120.13 131.55
	4011 4012	0	ILE B	11 12	0 45.7	700	90.761 90.162	2.448 2.952	1.00 1.00	131.55
	4013 4014	N CA	TYR B	12 12			89.457	4.286 4.186		143.62 143.62
30	4015 4016	CB	TYR B			550 935	88.215 88.292	4,258 4,175	1.00	143.62
	4017 4018	CD1 CE1	TYR B	12	20 47.	.725 .966	87.153 86.963	4.019 3.93	1.00	143.62 143.62
35	4019	CD2 CE2	TYR B	1	20 45	.733 .117	85.821 85.918	4.01	1.00	143.62
Э.	4021	CZ OH	TYR B	. 1	20 47	.898	84.776 91.304	3.93 3.14	6 1.00	131.55
	4022 4023	c o	TYR B	1	20 43	3.506 3.919	92.426 91.024	3.39 3.01	3 1.0	0 134.10
4	4024 () 4025	N	TYR E		121 4	2.221 1.210	92.047 92.433	3.19 1.86		0 128.02
	4026 4027	CA CB	TYR I	3	121 4 121 4	0.572 1.444	93.147	0.84 0.44	36 1.0	ທ 128.02
	4028 4029	CG CD1	TYR	B	121 4	2.598 3.370	92.562 93.184	-0.6	12 1.0	იი 128.02
4	4030 4031	CE1 CD2	TYR TYR	В	121 4	1.060 11.810	94.376 95.003	0.3 -0.6	81 1.0	00 128.02 00 128.02
	4032	CE2 CZ	TYR TYR	В	121 4	<u> 12.970</u>	94.395 94.979	-1.1 -2.1	55 1.	00 128.02
	4033 4034	OH	TYR	B B	121	43.710 40.085	91.591 90.483	4.0	39 1.	.00 134.10
	50 4035 4036	C O	TYR LYS	В	122	39.556 39.716	92.457 92.165		013 1	.00 124.90 .00 124.90
	4037 4038	N CA	LYS LYS	B	122 122	38.635 39.152	92.121	7.	442 1	.00 161.09 .00 161.09
	4039 55 4040	CG	LYS	В	122 122	38.059 38.511	91.814 92.092	9.	R42 1	1.00 161.09 1.00 161.09
	4041 4042	CD	LYS LYS	В	122 122	37.370 37.815	91.925 92.313	12	.166	1.00 161.09 1.00 124.90
	404: 404:	3 NZ	LYS	В	122	37.606 37.892	93.289 94.448	€	.146	1.00 124.90 1.00 160.91
	60 404	5 0	LYS ASF	• В	122 123	36.409	92.939 93.908		.250	1.00 160.91
	404 404	7 C/	ASI	Р В Р В	123 123	35.338 34.877	94.474 93.486		3.591 7.385	1.00 179.88
	404 404	i9 C	AS AS	PB PB	123 123	34.061 33.105	92.913	J.	6.817 8.583	1.00 179.88 1.00 179.88
	65 405 405	51 0	D2 AS	P B	123 123	34.365 35.719	93.289 95.056	, 5	4.324 4.671	1.00 160.91 1.00 160.91
	40 40	53 C	AS	PB	123 124	35.556 36.231	96.222 94.71	В	3.144 2.160	1.00 138.47 1.00 138.47
	40	54 N	A GI	Y B	124	36.604	95.72	8	£. 100	

. [

94.A

				401	37.853	96.561	2.426	1.00	138.47
	4056	С		124	37.653 38.295	97.314	1.543	1.00	138.47
	4057	0		124 125	38.430	96.420	3.621	1.00	138.22
	4058	N		125	39.627	97.166	4.009	1.00	138.22
_	4059	CA		125	39.534	97.532	5.496	1.00	228.57 228.57
5	4060	CB CG	GLU B	125	38.461	98.543	5.849 5.425	1.00 1.00	228.57 228.57
	4061	CD	GLU B	125	38.835	99.938	5.952	1.00	228.57
	4062 4063	OE1	GLU B	125	39.838	100.460 100.515	4.567	1.00	228.57
	4064	OE2	GLU B	125	38.132	96.411	3.763	1.00	138.22
10	4065	С	GLU B	125	40.934 41.001	95.195	3.933	1.00	138.22
	4066	0	GLU B	125 126	41.974	97.132	3.360	1.00	132.93
	4067	N.	ALA B ALA B	126	43.266	96.495	3.155	1.00	132.93 135.56
	4068	CA	ALA B	126	44.225	97.478	2.531	1.00	132.93
	4069	CB C	ALA B	126	43.730	96.115	4.563	1.00 1.00	132.93
15	4070	ŏ	ALA B	126	43.549	96.898	5.489 4.751	1.00	121.91
	4071 4072	Ň	LEU B	127	44.325	94.941 94.563	6.102	1.00	121.91
	4073	CA	LEU B	127	44.734	93.352	6.540	1.00	110.11
	4074	СВ	LEU B	127	43.939 43.777	93.371	8.046	1.00	110.11
20	4075	CG	LEU B	127 127	43.167	94.684	8.464	1.00	110.11
	4076	CD1	LEU B LEU B	127	42.902	92.200	8.476	1.00	110.11
	4077	CD2	LEU B	127	46.214	94.312	6.354	1.00 1.00	121.91 121.91
	4078	C O	LEU B	127	46.818	94.960	7.211 5.643	1.00	133.29
25	4079	N	LYS B	128	46.781	93.344	5. 77 9	1.00	133.29
23	4080 4081	ĊA	LYS B	128	48.199	93.025 91.693	6.524	1.00	231.48
	4082	CB	LYS B	128	48.384	91.675	7.942	1.00	231.48
	4083	CG	LYS B	128	47.832 48.657	92.524	8.899	1.00	231.48
	4084	CD	LYS B	128 128	48.119	92.423	10.322	1.00	231.48
30	4085	CE	LYS B LYS B	128	49.040	93.021	11.325	1.00	231.48 133.29
	4086	NZ	LYS B	128	48.770	92.918	4.365	1.00 1.00	133.29
	4087	C O	LYS B	128	48.009	92.760	3.392 4.243	1.00	155.64
	4088 4089	Ň	TYR B	129	50.095	92.99 9 92.894	2.930	1.00	155.64
35	4090	CA	TYR B	129		94.261	2.262	1.00	155.17
33	4091	CB	TYR B	129		94.324	1.124	1.00	155.17
	4092	CG	TYR B	129 129		93.892	-0.149	1.00	155.17
	4093	CD1	TYR B TYR B	129		93.900	-1.184	1.00	155.17 155.17
40	4094	CE1 CD2	TYR B	129		94.765	1.340	1.00 1.00	155.17
40	4095	CE2	TYR B	129		94.775	0.315 -0.950	1.00	155.17
	4096 4097	CZ	TYR B	129		94.340	-1.976	1.00	155.17
	4097	OH	TYR B	129		94.360 92.321	2.965	1.00	155.64
	4099	C	TYR B	129		92.644	3.857	1.00	155.64
45	4100	0	TYR B	12 13		91.477	1.982	1.00	137.92
	4101	N	TRP B	13		90.873	1.883	1.00	137.92 181.18
	4102	CA	TRP B	13		89.553	2.659	1.00	181.18
	4103	CB	TRP B	13	0 53.301	89.553	4.048		181.18
50	4104) 4105	CD2	TRP B	13		89.540	5.275 6.329		181.18
)(4106	CE2	TRP B	13		89.489 89.564	5.588		181.18
	4107	CE3	TRP B	13		89.516	4.397		181.18
	4108	CD1	TRP B	13	30 51.843	89.470	5.767		181.18
	4109	NE1	TRP B		30 53.470	89.458	7.667		181.18 181.18
5		CZ2	TRP B		30 55.778	89.532	6.928		181.18
	4111	CZ3 CH2	TRP B		30 54.816	89.490	7.949 0.42		137.92
	4112	C	TRP B	1	30 54.173	90.577	-0.48		137.92
	4113 4114	ŏ	TRP B		30 53.340	90.655 90.218	0.22	·	207.31
6	0 4115	Ň	TYR B		31 55.439		-1.10		207.31
·	4116	CA	TYR B		31 55.946 31 57.427		-1.19	8 1.00	239.97
	4117	CB	TYR B		31 57.427 31 57.952	454	-2.60		239.97
	4118	CG	TYR B		31 57.608		-3.53		239.97 239.97
	4119	CD1 CE1	TYR B		31 58.061	91.065	-4.84		239.97
•	5 4120	CD2	TYR E		131 58.768	89.101	-3.02		239.97
	4121	CE2	TYR E	3	131 59.226		-4.32 -5.23		239.97
	4122 4123	CZ	TYR E	3	131 58.871		-6.5°		239.97
	4124	OH	TYR E	3	131 59.314		-1.20		207.31
•	70 4125	С	TYR	3	131 55.74	, 60.001			

						87.903	-1.669	1.00	207.31
	4400	0			54.695	87.590	-0.805	1.00	245.95
	4126	Ň	GLU B		56.760	86.133	-0.780	1.00	245.95
	4127 4128	CA	GLU B		56.632	85.470	-0.236	1.00	249.39
	4129	СВ	G20 -	132	57.906 50.071	85.349	-1.220	1.00	249.39
5	4130	CG		132	59.071 59.448	83.901	-1.491	1.00	249.39 249.39
,	4131	CD		132 132	58.976	83.011	-0.751	1.00 1.00	249.39
	4132	OE1		132	60.223	83.649	-2.438	1.00	245.95
	4133	OE2	GLU B	132	55.535	86.097	0.271 1.341	1.00	245.95
	4134	CO	GLU B	132	55.697	86.700	0.003	1.00	176.11
10	4135	N	ASN B	133	54.430	85.403 85.462	0.965	1.00	176.11
	4136	CA	ASN B	133	53.339	84.935	0.335	1.00	160.36
	4137 4138	CB	ASN B	133	52.010 51.822	83.434	0.412	1.00	160.36
	4139	CG	ASN B	133 133	52.741	82.660	0.161	1.00	160.36 160.36
15	4140	OD1	ASN B ASN B	133	50.589	83.015	0.716	1.00 1.00	176.11
	4141	ND2	ASN B	133	53.555	84.965	2.388 2.802	1.00	176.11
	4142	C	ASN B	133	54.665	84.633	3.151	1.09	182.29
	4143	O N	HIS B	134	52.479	84.9 9 7	4.534	1.00	182.29
20	4144	CA	HIS B	134	52.525	84.611 85.860	5.391	1.00	249.69
20	4145 4146	СВ	HIS B	134	52.743	85.559	6.845	1.00	249.69
	4147	CG	HIS B	134	53.003 52.286	85.883	7.951	1.00	249.69 249.69
	4148	CD2	HIS B	134 134	54.081	84.836	7.264	1.00	249.69 249.69
	4149	ND1	HIS B	134	54.036	84.709	8.595	1.00 1.00	249.69
25	4150	CE1	HIS B HIS B	134	52.961	85.335	9.023 4.873	1.00	182.29
	4151	NE2	HIS B	134	51.200	83.948	3.984	1.00	182.29
	4152	C O	HIS B	134	50.446	83.556 83.832	6.163	1.00	162.56
	4153 4154	Ň	ASN B	135	50.922	83.206	6.644	1.00	162.56
30	4155	CA	ASN B	135	49.712	81.712	6.908	1.00	240.35
30	4156	СВ	ASN B	135	49.964 50.213	80.928	5.625	1.00	240.35 240.35
	4157	CG	ASN B	135 135		81.111	4.647	1.00 1.00	240.35
	4158	OD1	ASN B	135	51.216	80.048	5.620 7.919	1.00	162.56
	4159	ND2	ASN B	135	49.252	83.905	9.028	1.00	162.56
35	4160	C	ASN B	135		83.439 85.024	7.745	1.00	151.20
	4161 4162	Ň	ILE B	136		85.840	8.846	1.00	151.20
	4163	ĊA	ILE B	136		86.737	8.329	1.00	153.45
	4164	CB	ILE B	136 136		85.891	7.675	1.00	153.45 153.45
40		CG2	ILE B	130		87.526	9.477		153.45
	4166	CG1	ILE B	13		88.386	9.042 10.063		151.20
	4167	CD1 C	ILE B	13	6 47.495	85.052	10.003		151.20
	4168	ŏ	!LE B	13		84.466 85.084	11.133		137.33
4	4169 5 4170	Ň	SER B	13		84.351	12.353	1.00	137.33
-	4171	CA	SER B	13		83.553	12.782		185.84 185.84
	4172	CB	SER B	13 13		82.999	14.062		137.33
	4173	OG	SER B	13		85.154	13.549		137.33
_	4174	C	SER B		7 47.862	86.294	13.764 14.34		147.08
5	0 4175	0 N	ILE B		38 46.641	84.509	15.52		147.08
	4176	ČA	ILE B	13	38 46.043		15.24		140.24
	4177 4178	CB	ILE B	_	38 44.592	AC 000	16.54	4 1.00	140.24
	4179	CG2	ILE B		38 43.867 38 44.581	00.700	14.30		140.24 140.24
4	55 4180	CG1	ILE B		38 44.581 38 43.214	~~ ~~	13.73		147.08
	4181	CD1	ILE B		38 46.047	7 84.165	16.72		147.08
	4182	C	ILE B		38 45.49	4 83.059	16.67 17.80		249.69
	4183	O N	THA B	•	39 46.66		19.0		249.69
	4184	CA	THR B		139 46.76		19.8		249.31
	60 4185 4186	CB	THR B	3 '	139 47.94		20.0	34 1.00	249.31
	4187	OG1	THR E	3	139 47.80 139 49.25	~ ~~~	19.1	22 1.00	249.31 249.69
	4188	CG2	THR E	_	139 49.25 139 45.47		19.8		040.00
	4189	Ç	THR		139 44.59	20.450	19.7		4== 06
	65 4190	0	THR I	_	140 45.36	32 85.121	20.5		177.26
	4191	N	ASN	_	140 44.2	11 85.439	21.3 22.5		040.00
	4192		ASN	В	140 44.6	~~ ~~ 4			249.69
	4193 4194		ASN	В	140 43.4				
	70 4195			В	140 42.4	22 01.240			
	70 7.00								

						aa ca4	24.665	1.00	249.69
_	1196	ND2		140	43.566	86.631 86.161	20.396	1.00	177.26
	1190 1197	C	,	140	43.247	87.200	19.812	1.00	177.26
	4198	Ŏ:	,,,,,,	140	43.59 6 42.040	85.615	20.236	1.00	147.92
	4199	N .	,. <u> </u>	141	41.050	86.199	19.327	1.00	147.92
	4200	CA		141 141	40.337	85.085	18.551	1.00	170.82
	4201	СВ	ALA B	141	40.015	87.128	19.967	1.00	147.92 147.92
	4202	C	ALA B ALA B	141	39.333	86.783	20.942	1.00 1.00	150.18
	4203	O N	THR B	142	39.910	88.316	19.389 19.840	1.00	150.18
	4204	CA	THR B	142	38.966	89.325	19.549	1.00	194.09
10	4205 4206	CB	THR B	142	39.487	90.741 90.870	20.055	1.00	194.09
	4207	OG1	THR B	142	40.823	91.777	20.202	1.00	194.09
	4208	CG2	THR B	142	38.595 37.681	B9.119	19.053	1.00	150.18
	4209	С	THR B	142 142	37.682	88.485	17.996	1.00	150.18
15	4210	0	THR B VAL B	143	36.580	89.650	19.560	1.00	151.70 151.70
	4211	N	VAL B	143	35.325	89.489	18.859	1.00 1.00	138.48
	4212	CA CB	VAL B	143	34.128	89.829	19.752 19.973	1.00	138.48
	4213	CG1	VAL B	143	34.053	91.341 89.308	19.122	1.00	138.48
20	4214 4215	CG2	VAL B	143	32.853	90.418	17.658	1.00	151.70
20	4216	Ċ	VAL B	143	35.313 34.595	90.168	16.688	1.00	151.70
	4217	0	VAL B	143 144	36.106	91.488	17.716	1.00	158.91
	4218	N .	GLU B GLU B	144	36.149	92.427	16.609	1.00	158.91 246.81
	4219	CA	GLU B	144	36.870	93.708	16.996	1.00 1.00	246.81
25	4220	CB CB	GLU B	144	36.208	94.445	18.127	1.00	246.81
	4221	CD	GLU B	144	37.054	94.424	19.371 19.317	1.00	246.81
	4222 4223	OE1	GLU B	144	38.183	94.958 93.872	20.396	1.00	246.81
	4223 4224	OE2	GLU B	144		91.811	15.407	1.00	158.91
30	4225	C	GLU B	144		92.346	14.312	1.00	158.91
50	4226	0	GLU B	144 145		90.676	15.606	1.00	116.08 116.08
	4227	N.	ASP B	145		89.992	14.501	1.00 1.00	169.83
	4228	CA	ASP B	145		88.943	15.039 15.570	1.00	169.83
25	4229	CB CG	ASP B	145	40.399	89.560	14.797	1.00	169.83
35	4230 4231	OD1	ASP B	145		90.286 89.327	16.756	1.00	169.83
	4232	OD2	ASP B	145		89.332	13.575	1.00	116.08
	4233	С	ASP B	14		88.992	12.450	1.00	116.08
	4234	0	ASP B SER B	14! 14		89.161	14.054	1.00	118.95 118.95
40	4235	N	SER B SER B	14	- · · ·	88.538	13.267	1.00 1.00	193.19
	4236	CA CB	SER B	14		88.361	14.116 15.261	1.00	193.19
	4237	OG	SER B	14	6 33.830	87.569	12.048	1.00	118.95
	4238 4239	č	SER B	14		89.394 90.591	12.186		118.95
45	4240	Ō	SER B	14		88.787	10.863	1.00	175.20
45	4241	N	GLY B	14		89.543	9.668		175.20 175.20
	4242	CA	GLY B		47 34.150 47 34.222	88.715	8.406		175.20
	4243	C	ULY B		47 34.162	87.487	8.467		119.45
E C	4244	0 N	THR B		48 34.350	89.383	7.260 5.967		119.45
50) 4245 4246	CA	THR B	1.	48 34.445	88.68 9 89.059	5.05		97.36
	4247	CB	THR B		48 33.224	00.000	4.11		97.36
	4248	* OG1	THR B		48 33.606 48 32.069		5.90		97.36
	4249	ÇG2	THR B		48 32.069 48 35.802		5.25		119.45 119.45
5	5 4250	C	THR B		48 36.102		4.83		115.49
	4251	0 N	TYR B		49 36.618	87.934	5.13 4.52		115.49
	4252	CA	TYR B		149 37.918		5.38		121.92
	4253 4254	CB	TYR B	•	149 38.966		6.83		121.92
6	0 4255	CG	TYR B		149 39.07		7.77		121.92
·	4256	CD1	TYR E		149 38.12 149 38.25		9.10	1.00	121.92
	4257	CE1	TYR E		149 38.25 149 40:15	~	7.20		121.92 121.92
	4258	CD2	TYR E	-	149 40.29		8.5		121.92
	4259	CE2	TYR		149 39.34	6 88.509	9.4		121.92
6	55 4260	CZ OH	TYR	В	149 39.50	1 88.875	10.8 3.1		115.49
	4261 4262	C	TYR		149 38.02		2.6		115.49
	4263	ŏ	TYR	В	149 37.18		2.4	02 1.00	
	4264	N	TYR	В	150 39.09 150 39.49	07 467		42 1.00	105.13
•	70 4265	CA	TYR	O					

.

, 14 (d) k

	4266 4267	CB CG CD1.	TYR B	150 150	38.454 38.643 39.713	88.037 89.480 89.864 91.204	0.005 -0.407 -1.214 -1.645	1.00 1.00 1.00 1.00	148.24 148.24 148.24 148.24
	4268 4269 4270 4271	CE1 CD2 CE2 CZ	TYR B	150 150 150 150	39.871 37.724 37.867 38.946	90.461 91.803 92.168 93.473	-0.031 -0.454 -1.268 -1.715	1.00 1.00 1.00 1.00	148.24 148.24 148.24 148.24
10	4272 4273 4274 4275	OH C O N	TYR B TYR B TYR B CYS B	150 150 150 151	39.096 40.836 41.228 41.612	88.014 89.015 87.372 87.840	0.809 1.414 -0.057 -0.332	1.00 1.00 1.00 1.00	105.13 105.13 132.14 132.14
	4276 4277 4278 4279	CA C O	CYS B CYS B CYS B	151 151 151 151	42.986 43.242 42.511 44.018	88.046 87.547 86.847	-1.822 -2.671 0.236 -0.462	1.00 1.00 1.00 1.00	132.14 132.14 149.67 149.67
15	4280 4281 4282 4283	CB SG N CA	CYS B THR B THR B	151 152 152 152	43.926 44.288 44.661 44.403	85.150 88.798 89.083 90.547	-2.129 -3.516 -3.887	1.00 1.00 1.00	118.50 118.50 151.99 151.99
20	4284 4285 4286 4287	CB OG1 CG2 C	THR B THR B THR B	152 152 152	45.395 43.014 46.154 46.951	91.385 90.976 88.854 89.115	-3.266 -3.430 -3.689 -2.768	1.00 1.00 1.00 1.00	151.99 118.50 118.50
25	4288 4289 4290 4291	O N CA C	THR B GLY B GLY B GLY B	152 153 153 153	46.544 47.956 48.309	88.378 88.132 87.906 87.747	-4.864 -5.089 -6.545 -7.387	1.00 1.00 1.00 1.00	134.78 134.78 134.78 134.78
20	4292 4293 4294	O N CA CB	GLY B LYS B LYS B LYS B	153 154 154 154	47.419 49.605 50.077 51.115	87.885 87.673 88.730 88.679	-6.842 -8.199 -8.542 -9.971	1.00 1.00 1.00 1.00	183.95 183.95 202.68 202.68
30	4295 4296 4297 4298	CG CD CE NZ	LYS B LYS B LYS B LYS B	154 154 154 154	52.591 53.158 54.131	89.815 89.756 90.860	-10.237 -11.649 -11.921 -8.377	1.00 1.00 1.00 1.00	202.68 202.68 202.68 183.95
35	4299 4300 4301 4302	C O N CA	LYS B LYS B VAL B VAL B	154 154 155 155	51.657 5 50.048	86.268 85.900 85.484 84.117	-7.729 -9.253 -9.558 -9.620	1.00 1.00 1.00 1.00	183.95 214.72 214.72 178.34
40	4306	CB CG1 CG2	VAL B VAL B VAL B VAL B	15! 15! 15: 15	5 49.717 5 48.581	83.155 81.766 83.118 84.193	-10.018 -8.276 -10.931	1.00 1.00 1.00 1.00	178.34 178.34 214.72 214.72
45	4307 4308 4309 4310	C O N CA	VAL B TRP B TRP B	15 15 15	5 50.530 6 52.321 6 53.050	84.738 83.636 83.695 83.105	-11.865 -11.061 -12.334 -13.514	1.00 1.00 1.00	210.74 210.74 249.69 249.69
	4311 4312 4313 4314	CB CG CD2 CE2	TRP B TRP B TRP B	15 15 15	56 51.997 56 52.972 56 52.277	81.615 80.576 79.346 80.563	-13.504 -13.670 -13.606 -13.864	1.00 1.00 1.00	249.69 249.69 249.69 249.69
50	0 4315 4316 4317 4318	CE3 CD1 NE1 CZ2	TRP B TRP B TRP B TRP B	1. 1 1	56 50.790 56 50.950 56 52.925	80.988 79.628 78.114 79.336	-13.35° -13.41¢ -13.72 -13.99	4 1.00 9 1.00 0 1.00	249.69 249.69 249.69
5	4319 5 4320 4321 4322	CZ3 CH2 C O	TRP B TRP B TRP B TRP B	1	56 54.285 156 53.249 156 54.162	78.129 85.183 85.808	-13.91 -12.59 -12.05 -13.40	5 1.00 9 1.00	249.69 210.74 210.74 156.28
(4323 4324 50 4325	N CA CB CG	GLN B GLN B GLN B GLN B	3 3	157 52.355 157 52.406 157 53.203 157 54.718	87.144 87.338 87.195	-13.76 -15.07 -14.9 -14.0	74 1.00 10 1.00	156.28 249.69 249.69 249.69
	4326 4327 4328 4329 65 4330 4331	CD OE1 NE2 C	GLN E GLN E GLN E GLN E GLN E	3 3 3 8 8 8	157 55.327 157 55.277 157 55.90 157 51.03 157 50.89	7 89.465 6 87.860 5 87.808 3 88.830	-14.3 -12.8 -13.8 -14.5 -13.2	40 1.00 93 1.00 91 1.00 65 1.00 43 1.00	
	4331 4332 4333 4334 70 4335	N CA CB CG	LEU LEU	B B B	158 50.02 158 48.69 158 47.74 158 47.84	8 87.836 87.025	-13.2 -14.1 -15.6	67 1.00 56 1.00	204.79 162.40

	CD	n LEU	в 158	46.441	87.082	-16.258 -16.037	1.00 1.00	162.40 162.40
4336	·			48.464	88.518	-16.037 -11.852	1.00	204.79
4337		LEU		48.124	87.959	-11.852	1.00	204.79
4338	_	LEU		48.450	87.172	-11.648	1.00	211.13
4339 5 4340		ASP	В 159	47.277	88.961 89.179	-10.351	1.00	211.13
4341		ASP	В 159	46.669	90.659	-10.178	1.00	203.85
4342		ASF	B 159	46.316	91.574	-10.416	1.00	203.85
434		g asf		47.491	91.461	-9.680	1.00	203.85
434		D1 ASF	B 159	48.489	92.407	-11.342	1.00	203.85
10 434	5 O		B 159	47.413 45.397	88.344	-10.208	1.00	211.13
434	6 C			44.695	88.096	-11.193	1.00	211.13
434	7 0		_	45.101	87.907	-8.984	1.00	157.46 157.46
434				43.891	87.12 9	-8.729	1.00	182.37
434				44.174	85.638	-8.836	1.00 1.00	182.37
15 435		B TY		44.781	85.232	-10.147 -10.315	1.00	182.37
· 435		in TY	R B 160	46.161	85.213	-11.517	1.00	182.37
435 435	-	E1 TY	RB 160	46.733	84.810 4.849	-11.217	1.00	182.37
435		D2 TY	R & 160		84.446	-12.433	1.00	182.37
20 43	• •	E2 TY	R B 160		84,423	-12.578	1.00	182.37
43		Z TY	R B 160		83.987	-13.765	1.00	182.37
43	57	OH TY			87.423	-7.372	1.00	157.46
43	58 (TY	'R B 160		87.686	-6.377	1.00	157.46
43	59 ('R B 160 JUB 161		87.358	-7.357	1.00	159.09 159.09
25 43			UB 161 LUB 161		87.625	-6.168	1.00	208.73
43			LU B 16		88.664	-6.527	1.00	208.73
			LU B 16		89.081	-5.420	1.00 1.00	208.73
	~~		LU B 16		90.353	-5.7 6 9 -5.169	1.00	208.73
20 43	,,,,,	OE1 G	LU B 16	1 37.289	90.587	-6.633	1.00	208.73
	,00	OF2 G	LUB 16	1 38.829	91.125	-5.703	1.00	159.09
	366 367	Č G	LU B 16		86.311 85.483	-6.531	1.00	159.09
	368	ō G	ILU B 16		86,120	-4.386	1.00	135.59
	369	N S	ER B 16		84.894	-3.798	1.00	135.59
	370		ER B 16		84.552	-2.508	1.00	156.53
	371		ER B 16	·	85.561	-1.523	1.00	156.53
4	372		SER B 16		85.022	-3.475	1.00	135.59 135.59
	373	_		32 37.948	86.125	-3.362	1.00	183.98
. 4	374		GLU B 10	63 37.785	83.891	-3.332	1.00 1.00	183.98
	375	• •		63 36.382	83.933	-2.974	1.00	249.53
	376	CA CB		63 35.794	82.514	-2.941 -4.311	1.00	249.53
	1377	CG	GLU B 1	63 35.543	81.880	-5. 03 0	1.00	249.53
	1378 1379	CD	GLU B 1	63 34.339	82.475 82.464	-4.456	1.00	249.53
	4380	OE1	GLU B 1	63 33.229	82,945	-6.173	1.00	249.53
	4381	OE2		63 34.498	84.544	-1.569	1.00	183.98
	4382	•		63 36.369 63 37.334	84,379	-0.818	1.00	183.98
	4383	_		163 37.334 164 35.304	85.273	-1,199		111.61
	4384	N		164 34.138	85.647	-2.030		194.84 111.61
50	4385	CD		164 35.206	85.903	0.122		194.84
	4386	CA		164 34.171	86.986	-0.090		194.84
	4387	CB CB		164 33.217	86.310	-1.015 1.197		111.61
	4388	C	PRO B	164 34.778	84.904	0.926		111.61
55	4389 4390	ŏ	PRO B	164 33.994		2.417		125.70
33	4391	Ň	LEU B	165 35.268		3.482		125.70
	4392	CA	LEU B	165 34.918	44	3.77		110.19
	4393	СВ	LEU B	165 38.104	450	4.86	в 1.00	110.19
	4394	CG	LEU B	165 35.906 165 34.494		4,80		110.19
60	4395	CD1	LEU B		04.070	4.71		110.19
	4396	CD2	LEU B	165 36.944 165 34.468		4.77		125.70 125.70
	4397	C	LEU B	165 35.12	7 85.716	5.27		120.14
	4398	0	ASN B	166 33.34	84.317	5.31		120.14
~~	4399	N CA	ASN B	166 32.80	9 84.855	6.57		189.75
65	4400	CA CB	ASN B	166 31.28		6.63 6.14		189.75
	4401 4402	ČĞ	ASN B	166 30.53		6.18		189.75
	4402 4403	OD1	ASN B	166 31.05		5.69		189.7
	4404	ND2	ASN B	166 29.30		7.7		120.14
70	4405	C	ASN B	166 33.42			•	
, 5								

4406 4407	7	Į.	ASN B ILE B ILE B	166 167 167	33.718 33.594 34.163	82.978 84.911 84.359	7.752 8.875 10.087 10.178	1.00 1.00 1.00 1.00	120.14 133.16 133.16 105.73
4408 4409	•	CB	ILE B	167	35.634	84.660 84.179	11.513	1.00	105.73
5 441	ŏ	CG2	ILE B	167 167	36.159 36.355	83.972	9.038	1.00	105.73 105.73
441	•	CG1	ILE B	167	37.820	84.256	9.039 11.319	1.00 1.00	133.16
441	_	CD1 C	ILE B	167	33.510	84.926 86.140	11.480	1.00	133.16
441 441	•	ŏ	ILE B	167	33.451	84.057	12.213	1.00	113.92
10 441	5	N	THR B	168 168	33.058 32.409	84.557	13.402	1.00	113.92 138.53
441	16	CA	THR B THR B	168	30.931	84.189	13.377	1.00 1.00	138.53
441	• •	CB OG1	THR B	168	30.347	84.678	12.163 14.563	1.00	138.53
44¹ 44¹	10	CG2	THR B	168	30.214	84.810 84.135	14.728	1.00	113.92
15 44		С	THR B	168 168	33.018 33.161	82.955	15.019	1.00 1.00	113.92 134.74
44		0	THR B VAL B	169	33.381	85.129	15.526 16.840	1.00	134.74
44		N CA	VAL B	169	33.953	84.905 85.795	17.049	1.00	119.12
	23 24	CB	VAL B	169	35.207 35.482	85.994	18.518	1.00	119.12
	25	CG1	VAL B VAL B	169 169	36.403	85.141	16.397	1.00 1.00	119.12 134.74
44	26	CG2	VAL B VAL B	169	32.864	85.249	17.868 18.047	1.00	134.74
	127	C	VAL B	169	32.511	86.415 84.222	18.527	1.00	162.52
	128 129	Ň	ILE B	170	32. 32 6 31.270	84.383	19.532	1.00	162.52 162.30
	430	CA	ILE B	170 170	30.271	83.207	19.449	1.00 1.00	162.30
4	431	CB CG2	ILE B	170	29.809	83.021	18.010 19.881	1.00	162.30
	432 433	CG1	ILE B	170		81.906 80.693	19.859	1.00	162.30
	433 434	CD1	ILE B	170 170		84.444	20.932	1.00	162.52 162.52
30 4	435	C	ILE B	170		84.092	21.122 21.923	1.00 1.00	183.47
· 4	436	0 Z	LYS B	171	31.114	84.869	23.278	1.00	183.47
	1437 1438	CA	LYS B	171		84.966 86.425	23.716		228.46 228.46
4	1439	CB	LYS B LYS B	171 17	·	87.040	23.602		228.46 228.46
	4440	CD	LYS B	17	1 30.316	88.539	23.398 24.538		228.46
	4441 4442	CE	LYS B	17			24.377	1.00	228.46
	4443	NZ	LYS B	17 17		-4404	24.319		183.47 183.47
	4444	C	LYS B Lys b	17		3 84,218	25.525		249.69
	4445	0 C1	NAG B	22	48.14		-2.146 -2.430		249.69
	4446 4447	C2	NAG B	22			-2.70	7 1.00	249.69 249.69
	4448	N2	NAG B NAG B	22	- ·	4 66.290	-2.51		249.69
	4449	C7 O7	NAG B		21 50.62	8 66.249	-2.11 -2.81		249.69
45	4450 4451	C8	NAG B		21 48.81		-3.61	4 1.00	249.69
	4452	C3	NAG B		21 50.11 21 51.25		-3.75		249.69 249.69
	4453	03	NAG B	_	21 50.56	38 61 <i>.</i> 956	-3.44 -4.71		249.69
50	4454	C4 O4	NAG B	2	21 51.1		-4.7 i		249.69
50	4455 4456	C5	NAG B	1 2	21 49.30 21 48.6		-1.9	12 1.00	249.69
	4457	O5	NAG E		221 48.6 221 49.7	51 59.637	-2.69		249.69 249.69
	4458	C6 O6	NAG E		221 50.7	00 59.612	-1.6 -4.7		249.69
55	4459 4460	C1	NAG E	3 7	222 51.9		-5.6	92 1.00	249.69
33	4461	C2	NAG E		222 53.1 222 53.9		-5.1		249.69 249.69
	4462	N2	NAG I NAG I	_	222 55.2	211 61.597			249.69
	4463	C7 O7	NAG	В	222 55.8				249.69
60	4464 4465	CB	NAG	В	222 55.9 222 52.0		'	123 1.00	249.69 249.69
00	4466	C3	DAN DAN		222 52.0 222 53.0		; -8.0	006 1.00	249.69
	4467	O3 C4	NAG		222 51.	697 59.96		668 1.00 900 1.00	249.69
	4468 4469	04 04	NAG	В		134 60.393 571 59.683	•	652 1.00	249.69
65	4470	C5	NAG	В		.571 59.68 .140 59.32	-5.	356 1.00	249.69 249.69
05	4471	O5	DAN DAN	р В		.642 58.55	1 -7.	.073 1.00 .979 1.00	
	4472	C6 O6	DAN		222 48	.276 58.93 .093 65.37		.979 1.00 .289 1.00	220.33
	4473 4474	C1	NAG	В	_	.093 65.37 2.619 64.78		.606 1.00	
70		C2	NAG	B	242 27	.019			

			NAC 5	040	28.439	63.617	-1.372	1.00	220.33
	4476	N2 ⊶	NAG B NAG B		28.079	62.446	-1.890	1.00	220.33
	4477	C7 O7	NAG B	242	27.061	62.304	-2.564	1.00	220.33
	4478	C8	NAG B	242	28.977	61,252	-1.616	1.00	220.33
5	4479 4480	æ	NAG B	242	28.417	65.869	-2.342	1.00	220.33
5	4481	03	NAG B	242	28.893	65.358	-3.579 -2.588	1.00 1.00	220.33 220.33
	4482	C4	NAG B	242	27.524	67.092	-2.306 -3.127	1.00	220.33
	4483	04	NAG B	242	28.320	68.165 67.565	-1.278	1.00	220.33
	4484	C5	NAG B	242 242	26.849 26.201	66.460	-0.583	1.00	220.33
10	4485	O5	NAG B NAG B	242 242	25.764	68.596	-1.552	1.00	220.33
	4486	C6 O6	NAG B	242	26.133	69.886	-1.090	1.00	220.33
	4487 4488	C1	NAG B	243	27.960	68.648	-4.371	1.00	233.97
	4489	C2	NAG B	243	28.552	70.043	-4.570 0.564	1.00 1.00	233.97 233.97
15	4490	N2	NAG B	243	28.067	70.964	-3.561 -2.911	1.00	233.97
	4491	C7	NAG B	243	28.929 30.147	71.745 71.719	-3.114	1.00	233.97
	4492	07	NAG B	243 243	28.358	72.696	-1.871	1.00	233.97
	4493	C8 C3	NAG B NAG B	243	28.185	70.544	-5.9 6 0	1.00	233.97
20	4494 4495	တ္သ	NAG B	243	28.726	71.840	-6.174	1.00	233.97
20	4496	C4	NAG B	243	28.751	69.586	-6.984	1.00	233.97 233.97
	4497	04	NAG B	243	28.443	70.118	-8.263 6.727	1.00 1.00	233.97
	4498	C5	NAG B	243	28.175	68.165	-6.727 -5.361	1.00	233.97
	4499	Q5	NAG B	243	28.488	67.756 67.113	-7.637	1.00	233.97
25	4500	C6	NAG B	243 243	28.776 30.175	66.991	-7.430	1.00	233.97
	4501	O6 C1	nag b Man b	243	29.240	69.921	-9.345	1.00	229.91
	4502 4503	C2	MAN B	244	28.260	69.705	-10.400	1.00	229.91
	4503 4504	02	MAN B	244	27.196	70.659	-10.238	1.00	229.91 229.91
30	4505	C3	MAN B	244	28.928	69.691	-11.752 -12.770	1.00 1.00	229.91
-	4506	03	MAN B	244	28.001	69.355 70.989	-12.013	1.00	229.91
	4507	C4	MAN B	244	29.658 30.237	70.964	-13.307	1.00	229.91
	4508	04 05	MAN B MAN B	244 244	30.732	71.128	-10.933	1.00	229.91
25	4509	C5 O5	MAN B	244	30.062	71.170	-9.601	1.00	229.91
35	4510 4511	6 6	MAN B	244	31.699	72.322	-11.158	1.00	229.91
	4512	06	MAN B	244	31.180	73.559	-10. 690	1.00	229.91 249.69
	4513	C1	NAG B	250	44,268	53.492	9.707 10.328	1.00 1.00	249.69
	4514	C2	NAG B	250	45.671	53.603 53.779	11.763	1.00	249.69
40	4515	N2	NAG B	250 250	45.573 45.937	52.792	12.578	1.00	249.69
	4516	C7 O7	NAG B NAG B	250	46.363	51.706	12.172	1.00	249.69
	4517 4518	C8	NAG B	250	45.811	53.044	14.074	1.00	249.69
	4519	ČŠ	NAG B	250	46.415	54.790	9.702	1.00	249.69 249.69
45	4520	03	NAG B	250	47.749	54.843	10.194 8.172	1.00 1.00	249.69
	4521	C4	NAG B	250	46.432	54.657 55.826	7.602	1.00	249.69
	4522	04	NAG B	250 250	47.008 44.994	54.460	7.640	1.00	249.69
	4523	C5	NAG B NAG B	250 250	44,369	53.324	8.287	1.00	249.69
50	4524 4525	O5 C 6	NAG B	250		54.206	6.139	1.00	249.69
30	4525 4526	0 6	NAG B	250		53.664	5.761	1.00	249.69
	4527	C1	NAG B	274		59.809	24.027 24.903	1.00 1.00	249.69 249.69
	4528	C2	NAG B	274		61.065	24.803 25.777	1.00	249.69
	4529	N2	NAG B	274		61.181 62.374	26.223	1.00	249.69
55	4530	C7	NAG B	274 274		63.422	25.934	1.00	249.69
	4531	O7 C8	NAG B	274		62.415	27.133	1.00	249.69
	4532 4533	cs	NAG B	274		60.997	25.741	1.00	249.69
	4534	03	NAG B	274		62.216	26.451	1.00 1.00	249.69 249.69
60	4535	C4	NAG B	274		60.745	24.836 25.637	1.00	249.69
	4536	04	NAG B	274		60.553 59.506	23.958	1.00	249.69
	4537	C5	NAG B	274		59.674	23.192	1.00	249.69
	4538	O5 C6	NAG B NAG B	274 274		59.255	22,962	1.00	249.69
65	4539 5 4540	O6	NAG B	27		58.209	22.054	1.00	249.69
U.	4540 4541	C1	NAG B	33	5 50.936	78.660	5.286	1.00	249.69 249.69
	4542	C2	NAG B	33		77.658	6.389 7.651	1.00 1.00	249.69
	4543	N2	NAG B	33		78.372 78.063	8. 66 8	1.00	249.69
. نبو	4544	C7	NAG B			77.166	8.611	1.00	249.69
70) 4545	07	NAG B	33	J 70.023	:			

								4.00	249.69
		00	NAG B	335	50.837	78.865	9.950	1.00 1.00	249.69
	4548	C8 C3	NAG B	335	52.711	76.938	6.115 6.909	1.00	249.69
	4547	03	NAG B	335	52.790	75.759 76.553	4.647	1.00	249.69
	4548 4549	C4	NAG B	335	52.852	75.970	4.410	1.00	249.69
5	4550	04	NAG B	335	54.131 52.678	77.814	3.812	1.00	249.69
,	4551	C5	NAG B	335 335	51.319	78.289	3.939	1.00	249.69
	4552	05	NAG B	335	52.935	77.564	2.334	1.00	249.69 249.69
	4553	C6	NAG B	335	53.923	78.447	1.826	1.00 1.00	249.69
4.0	4554	O6 C1	NAG B	340	43.529	87.808	25.515 26.379	1.00	249.69
10	4555	C2	NAG B	340	42.252	87.842 87.751	25.533	1.00	249.69
	4556 4557	N2	NAG B	340	41.073	86.909	25.835	1.00	249.69
	4558	C7	NAG B	340	40.086 40.099	86.177	26.8 33	1.00	249.69
	4559	07	NAG B	340 340	38.898	86.878	24.882	1.00	249.69 249.69
15	4560	C8	NAG B NAG B	340	42.235	89.153	27.182	1.00 1.00	249.69
	4561	C3	NAG B	340	41.117	89.172	28.061 27.991	1.00	249.69
	4562	O3 C4	NAG B	340	43.537	89.304	28.606	1.00	249.69
	4563	04	NAG B	340	43.566	90.587 89.134	27.069	1.00	249.69
20	4564 4565	C5	NAG B	340	44.768	87.8 7 7	26.352	1.00	249.69
20	4566	O 5	NAG B	340	44.691 46.101	89.143	27.805	1.00	249.69
	4567	C6	NAG B	340 340	47.172	88.783	26.936	1.00	249.69 212.59
	4568	Q 6	NAG B	366	28.566	86.792	5.084	1.00	212.59
	4569	C1	NAG B NAG B	366		86.264	3.928	1.00 1.00	212.59
25	4570	C2	NAG B	366		85.657	2.952 3.019	1.00	212.59
	4571	N2 C7	NAG B	366	28.903	84.360	3.883	1.00	212.59
	4572	O7	NAG B	366		83.623 83.792	1.966	1.00	212.59
	4573 4574	C8	NAG B	366		83.792 87.413	3.282	1.00	212.59
30		C3	NAG B	366		86.895	2.319	1.00	212.59
50	4576	O3	NAG B	366 366	·	88.236	4.315	1.00	212.59 212.59
	4577	C4	NAG B NAG B	366		89.443	3.682	1.00 1.00	212.59
	4578	04	NAG B	36		88.607	5.499	1.00	212.59
	4579	C5 O5	NAG B	36	6 27.723	87.423	6.036 6.648	1.00	212.59
35		C6	NAG B	36		89.288 89.790	7.613	1.00	212.59
	4581 4582	06	NAG B	36		89.710	3.786	1.00	243.26
	4583	C1	NAG B	36		91.194	3.541	1.00	243.26
	4584	C2	NAG B	36 36		92.006	4.472	1.00	243.26 243.26
4(N2	NAG B NAG B	36		92.768	4.025	1.00 1.00	243.26
	4586	C7 O7	NAG B	36	·	92.827	2.834 5.058		243.26
	4587	C8	NAG B	36	67 26.602	93.591	3.687		243.26
	4588 4589	cs	NAG B	_	67 22.591	91.455 92.825	3,445		243.26
4		03	NAG B		67 22.313 67 21.820	90.586	2.689		243.26
7	4591	C4	NAG B		67 21.820 67 20.423	90.749	2.897		243.26 243.26
	4592	04	NAG B NAG B		67 22.208	89.105	2.859		243.26
	4593	C5	NAG B	. 3	67 23.647	88.941	2.791		243.26
_	4594	O5 C6	NAG B	_	67 21.611	88.219	1.777 0.91		243.26
2	(O 4595 4596	06	NAG B	3	67 22.614	87.692 67.814	61.47		249.69
	4597	CB	LYS) 4	55.929	66.389	61.06	9 1.00	249.69
	4598	CG	LYS		4 55.569 4 55.219	65.523	62.28	0 1.00	249.69
	4599	CD	LYS		4 55.219 4 54.831	64.103	61.85		249.69 249.69
	55 4600	CE	LYS (LYS (-	4 54.503	63.215	63.02		226.67
	4601	ΝZ	LYS		4 54.982	68.782	59.37 59.81		226.67
	4602	C	LYS	Ď	4 53.862		60.76		226.67
	4603 4604	Ň	LYS	D	4 56.551		60.2		226.67
	60 4605	ČA	LYS	_	4 56.206		58.09	98 1.00	199.21
	4606	N	PRO		5 55.175 5 56.399		57.5		157.97 199.21
	4607	CD	PRO		5 56.399 5 54.056		57.1		4-7-07
	4608	CA	PRO PRO		5 54.55	70.184	56.1		467 67
	4609	CB	PRO		5 56.009	69.877	56.0		
	65 4610	CG C	PRO		5 53.74		56.5 56.5		199.21
	4611 4612	_	PRO		5 54.59		56.0		205.80
	4612 4613		LYS	D	6 52.52		55.4	468 1.00	205.80
	4614	, CA			6 52.13 6 51.39		56.4	489 1.00	249.69
	70 4615		LYS	U		• •			

					51,007	64.131	55.942	1.00	249.69
	4616	CG CG	LYS D Lys d	6 ·	50.433	63.220	57.018	1.00	249.69
	4617	CD CE	LYS D	6	50.116	61.838	56.448	1.00	249.69
	4618	NZ NZ	LYS D	6	49.665	60.880	57.497	1.00	249.69
5	4819 4620	C	LYS D	6	51.263	66.599	54.246	1.00	205.80
5	4621	ŏ	LYS D	6	50.132	67.075	54.362	1.00	205.80
	4622	Ñ	VAL D	7	51.797	66.245	53.080 51.823	1.00 1.00	180.35 180.35
	4623	CA	VAL D	7	51.082	· 66.425	50.636	1.00	112.97
	4624	CB	VAL D	7	52.002	66.148 66.692	49.350	1.00	112.97
10	4625	CG1	VAL D	7	51.369 53.374	66.752	50.884	1.00	112.97
	4626	CG2	VAL D VAL D	7 7	49.846	65.540	51.677	1.00	180.35
	4627	C	VAL D	7	49.935	64.315	51.772	1.00	180.35
	4628	0 N	SER D	8	48.699	66.171	51.443	1.00	191.62
15	4629 4630	CA	SER D	8	47.441	65.455	51.269	1.00	191.62
13	4631	CB	SER D	8	46.339	66.118	52.114	1.00	215.34 215.34
	4632	OG	SER D	8	46.315	67.528	51.940 49.790	1.00 1.00	191.62
	4633	С	SER D	8	47.066	65.475 66.285	49.026	1.00	191.62
	4634	O .	SER D	8	47.587 46.175	64.579	49.374	1.00	183.49
20	4635	N	LEU D LEU D	9 9	45.753	64.552	47.973	1.00	183.49
	4636	CA	LEU D	9	46.289	63.316	47.250	1.00	153.82
	4637	CB CG	LEU D	9	47.793	63.054	47.150	1.00	153.82
	4638 4639	CD1	LEU D	9	48.011	61.992	46.080	1.00	153.82
25	4639 4640	CD2	LEU D	9	48.557	64.312	46.800	1.00	153.82
23	4641	Č	LEU D	9	44.243	64.561	47.836	1.00	183.49 183.49
	4642	Ō	LEU D	9	43.522	64.243	48.781 46.650	1.00 1.00	161.08
	4643	N	ASN D	10	43.769	64.929 64.954	46.383	1.00	161.08
	4644	CA	ASN D	10	42.340 41.701	66.192	46.999	1.00	220.60
30	4645	CB	ASN D	10 10	40.195	66.089	47.052	1.00	220.60
	4646	CG OD1	ASN D ASN D	10	39.645	65.222	47.732	1.00	220.60
	4647	ND2	ASN D	10	39.515	66.966	46.328	1.00	220.60
	4648 4649	C	ASN D	10	42.077	64.931	44.883	1.00	161.08
35	4650	ŏ	ASN D	10	42.376	65.903	44.187	1.00	161.08 193.66
33	4651	Ň	PRO D	11	41.505	63.830	44.368 42.927	1.00 1.00	148.22
	4652	CD	PRO D	11	41.212	63.723 62.602	45.052	1.00	193.66
	4653	CA	PRO D	11	41.077	61.698	43.905	1.00	148.22
40	4654	CB	PRO D	11 11	40.656 40.146	62.658	42.901	1.00	148.22
40	4655	ÇG	PRO D PRO D	11	42.161	61.959	45.924	1.00	193.66
	4656	CO	PRO D	11	43.336	62.325	45.849	1.00	193.66
	4657 4658	N	PRO D	12	41.772	60.982	46.769	1.00	193.56
	4659	CD	PRO D	12	40.402	60.544	47.062	1.00	138.53 193.56
45	4660	CA	PRO D	12	42.731	60.293	47.644 48.588	1.00 1.00	138.53
	4661	CB	PRO D	12	41.824	59.503	48.520	1.00	138.53
	4662	CG	PRO D	12	40.494	60.225 59.379	46.825	1.00	193.56
	4663	Ç	PRO D	12	43. 63 3 44.775	59.096	47.204	1.00	193.56
	4664	0	PRO D TRP D	12 13	43.081	58.919	45.700	1.00	115.99
50	4665	N CA	TRP D	13	43.745	58.039	44.727	1.00	115.99
	4666	CB	TRP D	13	42.854	57.917	43.495	1.00	155.11
	4667 4668	ÇG	TRP D	13	41.432	57.624	43.839	1.00	155.11
	4669	CD2	TRP D	13	40.964	56.869	44.959	1.00	155.11 155.11
55	4670	CE2	TRP D	13	39.560	56.822	44.873	1.00 1.00	155.11
	4671	CE3	TRP D	13	41.596	56.233	46.022 43.138	1.00	155.11
	4672	CD1	TRP D	13	40.330	57.988 57.509	43.751	1.00	155.11
	4673	NE1	TRP D	13	39.192 38.778	56.160	45.808	1.00	155.11
	4674	CZ2	TRP D	13 13		55.569	46.957	1.00	155.11
60		CZ3 CH2	TRP D	13		55.538	46.844	1.00	155.11
	4876	C	TRP D	13		58.540	44.288	1.00	115.99
	4677 4678	ŏ	TRP D	13		59.565	43.618	1.00	115.99
	4676 4679	Ň	ASN D	14	46.176	57.810	44.644	1.00	127.73 127.73
65	4680	CA	ASN D	14		58.211	44.268 45.485	1.00 1.00	164.43
-	4681	СВ	ASN D	14		58.128	45.485 45.996	1.00	164.43
	4682	CG	ASN D	14		56.717 56.039	46.369	1.00	164.43
	4683	OD1	ASN D			56.265	46.023	1.00	164.43
_	4684	ND2	ASN D			57.395	43.094	1.00	127.73
70) 4685	С	ASN D		0.127				

						e7 001	42.929	1.00	127.73
4	686	0	ASN D	14	49.361	57.291 56.825	42.304	1.00	124.12
	687	N	ARG D	15	47.202 47.484	56.018	41.111	1.00	124.12
	1688	CA	ARG D	15	47. 404 47. 2 49	54.517	41.374	1.00	138.52
	1689	CB	ARG D	15 15	47.935	53.919	42.607	1.00	138.52
	1690	CG	ARG D	15	47.775	52.394	42.630	1.00 1.00	138.52 138.52
	4691	CD NE	ARG D	15	48.696	51.717	41.716 41.012	1.00	138.52
	4692 4692	CZ	ARG D	15	48.387	50.631	41.111	1.00	138.52
	4693 4694	NH1	ARG D	15	47.175	50.091 50.084	40.211	1.00	138.52
	4695	NH2	ARG D	15	49.292	56.487	40.117	1.00	124.12
	4696	С	ARG D	15	46.436 45.277	56.068	40.197	1.00	124.12
	4697	0	ARG D	15 16	46.825	57.344	39.182	1.00	134.05
	4698	N	ILE D ILE D	16	45.853	57.861	38.222	1.00	134.05 185.30
	4699	CA	ILE D	16	45.666	59. 359	38.405	1.00 1.00	185.30
15	4700	CB CG2	ILE D	16	44.824	59.635	39.645 38.464	1.00	185.30
	4701	CG1	ILE D	16	47.047	60.016	38.379	1.00	185.30
	4702 4703	CD1	ILE D	16	47.030	61.514 57.638	36.740	1.00	134.05
	4704	C	ILE D	16	46.150	57.474	36.330	1.00	134.05
20	4705	0	ILE D	16	47.301 45.088	57.650	35.944	1.00	221.22
	4706	N	PHE D	17 17	45.198	57.475	34.508	1.00	221.22
	4707	CA	PHE D PHE D	17	43.814	57.258	33.908	1.00	170.58 170.58
	4708	CB	PHE D	17	43.398	55.818	33.833	1.00 1.00	170.58
0.5	4709	CG CD1	PHE D	17	42.060	55.454	34.005 33.544	1.00	170.58
25	4710	CD2	PHE D	17	44.330	54.832	33,886	1.00	170.58
	4711 4712	CE1	PHE D	17	41.658	54.141 53.511	33.422	1.00	170.58
	4713	CE2	PHE D	17	43.932	53.167	33.594	1.00	170.58
	4714	CZ	PHE D	17	42.590 45.825	58.706	33.880	1.00	221.22
30	4715	С	PHE D	17	48.106	59.689	34.562	1.00	221.22
•	4716	0	PHE D LYS D	17 18	46.023	58.646	32.569	1.00	189.75 189.75
	4717	N	LYS D	18	46.615	59.743	31.808	1.00 1.00	249.69
	4718	CA CB	LYS D	18	47.255	59.178	30.538	1.00	249.69
25	4719	CG	LYS D	18	47.978	60.189	29.663 28.531	1.00	249.69
35	4720 4721	GD GO	LYS D	18	48.719	59.471 60.449	27.572	1.00	249.69
	4722	CE	LYS D	. 18	49.392	61,242	26.779	1.00	249.69
	4723	NZ	LYS D	18	48.405 45.573	60.806	31.450	1.00	189.75
	4724	С	LYS D	18 18	45.575 44.509	60.493	30.912	1.00	189.75 246.53
40	4725	0	LYS D GLY D	19	45.887	62.060	31.766	1.00	246.53 246.53
	4726	N	GLY D	19		63.151	31.467	1.00 1.00	246.53
	4727	GA Ç	GLY D	19		63.582	32.607 32.512	1.00	246.53
	4728 4729	Ö	GLY D	19		64.620	33.680	1.00	150.48
45	4730	Ň	GLU D	20		62.794 63.103	34.849	1.00	150.48
73	4731	CA	GLU D	20		61.840	35.704	1.00	195.02
	4732	СВ	GLU D	20 20		60.576	34.943		195.02
	4733	CG	GLU D	20		59.403	35.877		195.02 195.02
	4734	CD	GLU D	20		59.054	36.735		195.02
50		OE1 OE2	GLU D	2	41.093	58.831	35.748 35.717		150.48
	4736	C	GLU D	2	0 43.844	64.181	35.641		150.48
	4737 4738	ŏ	GLU D	2		64.375 64.870	36.545	1.00	166.05
	4739	Ň	ASN D	2		65.916	37.40		168.05
55	4740	CA	ASN D		1 43.621 1 42.869	67.242	37.24		249.69
	4741	CB	ASN D		1 42.869 1 42.390	67.487	35.82		249.69
	4742	ca	ASN D		43.129	67.337	34.85		249.69 249.69
	4743	OD1	ASN D		1 41.130	67.891	35.72		166.05
-	4744	ND2 C	ASN D		21 43.632	65.566	38.90 39.41		166.05
60		ŏ	ASN D		21 42.697		39.59		232.99
	4746 4747	Ň	VAL [) ;	22 44.685		41.02		232.99
	4747 4748	CA	VAL	-	22 44.836		41.27		144.01
	4749	СВ	VAL. I	_	22 45.811 22 47.232		40.94	1.00	144.01
6	5 4750	CG1	VAL	_	22 47.232 22 45.711		42.71		144.01 232.99
	4751	CG2	VAL VAL	_	22 45.367	7 67.003	41.7		232.99
	4752	C	VAL		22 46.13	2 67.762	41.13		149.70
	4753 4754	0 N	THR		23 44.97	7 67.204	42.9 43.7		149.70
-	4754 70 4755	CA	THR		23 45.40	9 68.376	40.7		
•	7,33	-			•				

					44.405	69.205	44.222	1.00	239.97
	4756	СВ	THR D	23 .	44.185 43.328	69.469	43.101	1.00	239.97
	4757	OG1	THR D	23	44.641	70.527	44.839	1.00	239.97
	4758	CG2	THR D	23 23	46.242	68.035	45.013	1.00	149.70
	4759	Ç	THR D	23	45.802	67.260	45.865	1.00	149.70 183.97
5	4760	0	LEU D	24	47.426	68.633	45.130	1.00 1.00	183.97
	4761	N	LEU D	24	48.291	68.390	46.282	1.00	149.27
	4762	CA CB	LEU D	24	49.736	68.117	45.847 44.528	1.00	149.27
	4763	CG	LEU D	24	50.067	67.414	44.556	1.00	149.27
10	4764 4765	CD1	LEU D	24	51.537	66.998 66.203	44.315	1.00	149.27
10	4766	CD2	LEU D	24	49.182	69.583	47.247	1.00	183.97
	4767	Ċ	LEU D	24	48.292	70.627	46.961	1.00	183.97
	4768	0	LEU D	24	48.884 47.642	69.414	48.394	1.00	179.50
	4769	N	THR D	25 25	47.555	70.453	49.422	1.00	179.50 206.28
15	4770	CA	THR D THR D	25	46.149	70.455	50.074	1.00 1.00	206.28
	4771	CB	THR D	25	45.152	70.641	49.059	1.00	206.28
	4772	OG1 CG2	THR D	25	46.035	71.567	51.109 50.510	1.00	179.50
	4773	C	THR D	25	48.608	70.207	50.983	1.00	179.50
20	4774	ŏ	THR D	25	48.762	69.083 71.258	50.907	1.00	232.65
20	4775 4776	Ň	CYS D	26	49.321	71.230	51.941	1.00	232.65
	4777	CA	CYS D	26	50.349	71.185	53.337	1.00	232.65
	4778	С	CYS D	26	49.723 48.767	71.928	53.562	1.00	232.65
	4779	0	CYS D	26 26	51.377	72.252	51.784	1.00	181.06 181.06
25	4780	CB	CYS D	26	52.866	72.078	52.815	1.00	211.42
	4781	SG	ASN D	27	50.274	70.400	54.266	1.00 1.00	211.42
	4782	N	ASN D	27	49.762	70.299	55. 633	1.00	249.69
	4783	CA CB	ASN D	27	50.909	70.245	56.640 58.041	1.00	249.69
20	4784	CG	ASN D	27	50.435	69.883	58.228	1.00	249.69
30	4785 4786	OD1 ·	ASN D	27	49.691	68.915 70.658	59.035	1.00	249.69
	4787	ND2	ASN D	27	50.866	71.397	56.027	1.00	211.42
	4788	С	ASN D	27	48.782 49.176	72.473	56.478	1.00	211.42
	4789	0	ASN D	27 28	47.499	71.096	55.848	1.00	232.09 232.09
35	4790	N	GLY D	28	46.428	72.024	56.166	1.00	232.09
	4791	CA	GLY D	28	45.145	71.413	55.640	1.00 1.00	232.09
	4792	C	· GLY D	28	45.028	71,150	54.442 56.527	1.00	249.69
	4793	0 N	ASN D	29	44.183	71.179	56,138	1.00	249.69
40	4794 4795	CA	ASN D	29		70.564 70.041	57.392	1.00	249.66
40	4796	СВ	ASN D	29		69.139	57.060	1.00	249.66
	4797	CG	ASN D	29		68.758	55.903	1.00	249.66
	4798	OD1	ASN D	29 29		68.786	58.082	1.00	249.66 249.69
	4799	ND2	ASN D	29		71.490	55.331	1.00	249.69
45		C	ASN D	29		71.122	54.239	1.00 1.00	249.69
	4801	O N	ASN D	3		72.692	55.843 55.146		249.69
	4802	CA	ASN D	3	0 40.830	73.606	55.941		249.69
	4803 4804	CB	ASN D	3		73.728 72.406	56.039		249.69
5		ÇĞ	ASN D			72.011	57.123		249.69
٠,	4806	OD1	ASN D		0 38.314 0 38.607	71.718	54.903		249.69
	4807	ND2	ASN D	_	38.607 30 41.378	75.001	54.827		249.69
	4808	Ç	ASN D		30 41.596	75.328	53.656		249.69 244.83
_	4809	0	PHE D		41.599	75.820	55.850		244.83
5	5 4810	N	PHE		31 42.085	77.179	55.63 56.23		249.48
	4811	CA CB	PHE C		31 41.091	78.191	55. 7 3		249.48
	4812	ca	PHE [31 39.675	78.021 77.036	56.26		249.48
	4813 4814	CD1	PHE	D :	31 38.843	1	54.70	_	249.48
•	50 4815	CD2	PHE		31 39.182	wa 0.40	55.78	2 1.00	249.48
`	4816	CE1	PHE	_	31 37.543 31 37.880		54.20		249.48
	4817	CE2	PHE	_			54.75		249.48 244.83
	4818	cz	PHE	_	31 37.061 31 43.496	77.454	56.16		244.83
	4819	C	PHE PHE		31 43.77	77.287	57.35		249.69
1	65 4820	0	PHE		32 44.37	3 77.888	55.2		249.69
	4821	N CA	PHE		32 45.77		55.59 54.79	• • • • • •	249.69
	4822 4823	CB	PHE	D	32 46.71		55.2		249.69
	4824	ČĞ	PHE	D	32 48.13		56.5		
	70 4825	CD.		D	32 48.43	5 70.710			

1 :

				32-	49.164	77.800	54.494	1.00	249.69
	4826	CD2	, , ,	32	49.752	76.678	56.983	1.00	249.69
	4827	CE1	PHE D	32	50.487	77.770	54.954	1.00	249.69
	4828	CE2	PHE D	32	50.779	77.207	56.198	1.00	249.69 249.69
_	4829	CZ	PHE D	32	46.086	79.681	55.325	1.00 1.00	249.69
5	4830	C	PHE D	32	45.300	80.381	54.671 55.802	1.00	237.86
	4831	N	GLU D	33	47.241	80.150	55.640	1.00	237.86
	4832 4833	CA	GLU D	33	47.603	81.555	57.029	1.00	249.69
	4834	CB	GLU D	33	47.766	82.184 83.708	57.034	1.00	249.69
10	4835	CG	GLU D	33	47.688	84.238	56.256	1.00	249.69
10	4836	CD	GLU D	33	46.478 45.351	83.734	56.476	1.00	249.69
	4837	OE1	GLU D	33 33	46.656	85.163	55.429	1.00	249.69
	4838	OE2	GLU D	33	48.821	81.908	54.779	1.00	237.86 237.86
	4839	Ç	GLU D	33	48.729	82.759	53.896	1.00	249.69
15	4840	0 N	VAL D	34	49.957	81.269	55.041 54.302	1.00 1.00	249.69
	4841	CA	VAL D	34	51.188	81.553	54.850	1.00	245.39
	4842 4843	CB	VAL D	34	52.357	80.686	54.126	1.00	245.39
	4844 4844	CG1	VAL D	34	53.648	81.015 80.928	56.343	1.00	245.39
20	4845	CG2	VAL D	34	52.522	81.386	52.773	1.00	249.69
20	4846	Ċ	VAL D	34	51.103 50.330	80.567	52.254	1.00	249.69
	4847	0	VAL D	34	51. 9 00	82.188	52.065	1.00	249.69
	4848	N	SER D	35 35	51.963	82.160	50.603	1.00	249.69
_	4849	CA	SER D	35	51.850	83.577	50.033	1.00	241.64 241.64
25	4850	СВ	SER D SER D	35	53.028	84.324	50.300	1.00	249.69
	4851	OG C	SER D	35	53.307	81.559	50.188	1.00 1.00	249.69
	4852	C	SER D	35	53.587	81.400	48.997 51.1 8 4	1.00	249.69
	4853 4854	Ň	SER D	36	54.137	81.243	50.953	1.00	249.69
30	485 4 4855	ĞA	SER D	36	55.455	80.654 81.325	51.841	1.00	249.69
30	4856	СВ	SER D	38	56.516	80.950	53.201	1.00	249.69
	4857	OG	SER D	36	56.379 55.430	79.150	51.227	1.00	249.69
	4858	С	SER D	36 36	55. 65 0	78.692	52.354	1.00	249.69
	4859	0	SER D THR D	37	55.147	78.389	50.176	1.00	216.36 216.36
35	4860	N	THR D THR D	37	55.091	76. 944	50.267	1.00 1.00	218.49
	4861	CA CB	THR D	37	53.651	76.439	50.029	1.00	218.49
	4862	OG1	THR D	37	52.773	77.009	51.009 50.138	1.00	218.49
	4863 4864	CG2	THR D	37	53.595	74.930	49.193	1.00	216.36
40		Č	THR D	37	56.027	76.399 76.908	48.070	1.00	216.36
40	4866	Ö	THR D	37	56.067	75.372	49.539	1.00	249.68
	4867	N	LYS D	38	56.792 57.737	74.790	48.591	1.00	249.68
	4868	CA	LYS D	38 38	59.115	74.638	49.265	1.00	248.74 248.74
	4869	CB	LYS D	38	59.701	75.962	49.786	1.00	248.74 248.74
45		CG	LYS D	38	61.060	75.782	50.467	1.00 1.00	248.74
	4871	CD CE	LYS D	38		77.123	50.933 51.599	1.00	248.74
	4872	NZ	LYS D	38	62.953	76.993	48.044	1.00	249.68
	4873 4874	Ċ	LYS D	38		73.445 72.660	48.747	1.00	249.68
50) 4875	ō	LYS D	38		72.000 73.197	46.775	1.00	200.98
٠,	4876	N	TRP D	39		71.944	46.137	1.00	200.98
	4877	CA	TRP D	39 39		72.188	45.096	1.00	193.49
	4878	CB	TRP D			72.634	45.638	1.00	193.49 193.49
_	4879	CG	TRP D			71.924	46.562		193.49
5.		CD2 CE2	TRP D			72.649	46.669 47.307		193.49
	4881	CE3	TRP D	_	9 54.053	70.747	47.307 45.247		193.49
	4882 4883	CD1	TRP D			73.727 73.745	45.854		193.49
	4884	NE1	TRP D) 3	9 52.822	73.745 72.242	47.487		193.49
6	0 4885	CZ2	TRP D		9 51.648	70.335	48.124	1.00	193.49
	4886	CZ3	TRP	-	19 52.994 19 51.807	71.084	48.20		193.49
	4887	CH2	TRP C	_		71.393	45.45		200.98
	4888	C	TRP (39 58.428 39 59.127	407	44.76		200.98 160.00
	4889	0	PHE 1		60 58.712	70.108	45.63		160.00
(55 4890	N CA	PHE	Ď 4	40 59.896	69.514	45.02 46.10		228.90
	4891	CB	PHE	_	40 60.943		46.10 46.93		228.90
	4892 4893	ÇĞ	PHE	D ·	40 61.397		47.99		228.90
	4894	CD1	PHE	D	40 60.620		46.67		228.90
•	70 4895	CD2	·· PHE	D	40 62.611	, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			
					•				

	4000	CE1	PHE D	40.	61.049	71.862	48.794	1.00	228.90
	4896	CE1 CE2	PHE D	40.	63.046	72.028	47.465	1.00	228.90
	4897 4898	CZ ·	PHE D	40	62.263	72.477	48.526	1.00	228.90
	4899	c	PHE D	40	59.620	68.2 6 6	44.183	1.00	160.00
5	4900	ŏ	PHE D	40	59.908	67.142	44.615	1.00	160.00
3	4901	Ň	HIS D	41	59.088	68.469	42.976	1.00	161.00
	4902	CA	HIS D	41	58.786	67.371	42.052	1.00	161.00
	4903	CB	HIS D	41	58.044	67.915	40.844	1.00	195.26
	4904	, CG	HIS D	41	57.679	66.868	39.847 38.493	1.00 1.00	195.26 195.26
10	4905	CD2	HIS D	41	57.680	66.881 65.626	40.216	1.00	195.26
	4906	ND1	HIS D	41	57.205 56.928	64.923	39.133	1.00	195.26
	4907	CE1	HIS D	41 41	57.207	65.660	38.073	1.00	195.26
	4908	NE2	HIS D HIS D	41	60.056	66.641	41.588	1.00	161.00
15	4909	C O	HIS D	41	60.798	67.153	40.751	1.00	161.00
13	4910 4911	N	ASN D	42	60.280	65.437	42.118	1.00	193.10
	4912	CA	ASN D	42	61.464	64.633	41.801	1.00	193.10
	4913	CB	ASN D	42	61.638	64.471	40.281	1.00	195.59
	4914	CG	ASN D	42	60.700	63.415	39.686	1.00	195.59
20	4915	OD1	ASN D	42	59.501	63.435	39.953 38.873	1.00 1.00	195.59 195.59
	4916	ND2	ASN D	42	61.240	62.506	42.397	1.00	193.10
	4917	Ç	ASN D	42	62.690	65.318 65.146	41.919	1.00	193.10
	4918	0	ASN D	42	63.810 62.462	66.092	43.456	1.00	217.79
05	4919	N	GLY D GLY D	43 43	63.540	66.809	44.120	1.00	217.79
25	4920	CA	GLY D	40 40	63.681	68.227	43.596	1.00	217.79
	4921 4922	C O	GLY D	43	63.883	69.166	44.372	1.00	217.79
	4923	Ň	SER D	44	63.567	68.373	42.275	1.00	249.69
	4924	CA	SER D	44	63.675	69.669	41.598	1.00	249.69
30	4925	CB	SER D	44	63.508	69.497	40.083	1.00	225.92
	4926	OG	SER D	44	64.485	68.631	39.546	1.00	225.92
	4927	С	SER D	44	62.620	70.652	42.085 41.997	1.00 1.00	249.69 249.69
	4928	0	SER D	44	61.423	70.374 71.806	42.579	1.00	241.20
	4929	N	LEV D	45	63.056 62.110	71.806 72.805	43.063	1.00	241.20
35	4930	CA	LEU D	45 45	62.841	74.084	43.488	1.00	237.73
	4931	CB CG	LEU D	45	61.948	75.186	44.070	1.00	237.73
	4932 4933	CD1	LEU D	45	61.151	74.631	45.239	1.00	237.73
	4934	CD2	LEU D	45	62.798	76.363	44.515	1.00	237.73
40	4935	č	LEU D	45	61.074	73.125	41.980	1.00	241.20
	4936	Ö	LEU D	45	61.365	73.051	40.783	1.00	241.20 233.99
	4937	N	SER D	46	59.865	73.470	42.416	1.00 1.00	233.99
	4938	CA	SER D	46	58.772	73.787	41.503 41.932	1.00	249.22
	4939	CB	SER D	46	57.494	73.050 73.250	40.995	1.00	249.22
45	4940	og .	SER D	46 46	56.444 58.506	75.285	41.441	1.00	233.99
	4941	C	SER D SER D	46	59.042	76.064	42.232	1.00	233.99
	4942 4943	0 N	GLU D	47	57.648	75.671	40.502	1.00	249.69
	4944 4944	CA	GLU D	47	57.306	77.074	40.285	1.00	249.69
50	4945	CB	GLU D	47	57.093	77.311	38.786	1.00	249.69
50	4946	CG	GLU D	47	58.330	77.026	37.945	1.00	249.69
	4947	CD	GLU D	47	58.089	77.248	36.471	1.00 1.00	249.69 249.69
	4948	OE1	GLU D	47	57.260	76.516	35.888 35.899	1.00	249.69
	4949	OE2	GLU D	47	58.728	78.156 77.618	41.063	1.00	249.69
55	4950	C	GLU D	47 47	56.102 55.889	78.827	41.111	1.00	249.69
	4951	0	GLU D	48	55.306	76.740	41.661	1.00	194.51
	4952 4953	N CA	GLU D	48	54.159	77.204	42.424	1.00	194.51
	4953 4954	CB	GLU D	48	53.081	76.117	42.492	1.00	249.69
60	4955	ČĞ	GLU D	48	51.885	76.488	43.366	1.00	249.69
O.	4956	CD	GLU D	48	51.102	<i>7</i> 7.675	42.836	1.00	249.69
	4957	OE1	GLU D	48	50.401	77.515	41.814	1.00	249.69 249.69
	4958	OE2	GLU D	48	51.189	78.768	43.437 43.826	1.00 1.00	194.51
	4959	Ç	GLU D	48	54.611	77.576	43.826 44.311	1.00	194.51
65	4960	0	GLU D	48	55. 64 5	77.100 78.438	44.472	1.00	208.13
	4961	N	THR D	49	53.834 54.134	78.889	45.831	1.00	208.13
	4962	CA	THR D	49 49	54.570	80.363	45.826	1.00	249.69
	4963	CB OG1	THR D	49	53.575	81.153	45.159	1.00	249.69
70	4964 4965	CG2	THR D	49	55.902	80.516	45.103	1.00	249.69
	-7000								

	49 6 6 49 6 7	C O	THR D	49	52.905 53.022 51.725	78.729 78.579 78.765	46.737 47.958 46.127	1.00 1.00 1.00	208.13 208.13 217.97
	4968	N.	ASN D ASN D		50.477	78.601	46.861	1.00	217.97
_	4969	CA	ASN D ASN D	50	49.294	78.643	45.885	1.00	202.82
5	4970	CB CB	ASN D	50	47.963	78.742	46.592	1.00	202.82 202.82
	4971	OD1	ASN D	50	47.874	78.441	47.781 45.865	1.00 1.00	202.82
	4972 4973	ND2	ASN D	50	46.924	79.156	45.665 47.545	1.00	217.97
	4974	C	ASN D	50	50.539	77.236 76.338	47.072	1.00	217.97
10	4975	Ö	ASN D	50	51.219	77.071	48.653	1.00	198.36
	4976	N	SER D	51 51	49.834 49.854	75.790	49.352	1.00	198.36
	4977	CA	SER D SER D	51	49.201	75.920	50.738	1.00	249.69
	4978	CB OG	SER D	51	47.794	76.051	50.640	1.00 1.00	249.69 198.36
15	4979	C	SER D	51	49.166	74.663	48.566 48.876	1.00	198.36
15	4980 4981	ŏ	SER D	51	49.350	73.484	47.555	1.00	249.63
	4982	Ň	SER D	52	48.375	75.019 74.019	46.739	1.00	249.63
	4983	CA	SER D	52	47.679 46.187	74.334	46.625	1.00	163.31
	4984	CB	SER D	52 52	45.563	74.298	47.891	1.00	163.31
20	4985	OG	SER D SER D	52	48.258	73.922	45.336	1.00	249.63 249.63
	4986	C	SER D	52	48.011	74.780	44.489	1.00 1.00	249.63 224.52
	4987	N	LEU D	53	49.024	72.867	45.096 43.799	1.00	224.52
	4988 4989	ČA	LEU D	53	49.637	72.642	43.799	1.00	138.37
25	4990	CB	LEU D	53	51.016	72.017 71.271	42.806	1.00	138.37
	4991	CG	LEU D	53	51.627 51.483	72.075	41.504	1.00	138.37
	4992	CD1	LEU D	53 53	53.089	70.983	43.128	1.00	138.37
	4993	CD2	LEU D	53	48.761	71.740	42.951	1.00	224.52 224.52
20	4994	C	LEU D	53	48.703	70.536	43.177	1.00 1.00	200.53
30	4995 4996	N	ASN D	54	48.080	72.325	41.973 41.115	1.00	200.53
	4990 4997	ČA	ASN D	54	47.219	71.538 72.402	40.513	1.00	228.73
	4998	СВ	ASN D	54	46.121	72.402 72.817	41.535	1.00	228.73
	4999	CG	ASN D	54 54	45.105 44.559	71.982	42.255	1.00	228.73
35	5000	OD1	asn d Asn d	54 54	44.839	74.111	41.608	1.00	228.73
	5001	ND2	ASN D	54	47.977	70.834	40.003	1.00 1.00	200.53 200.53
	5002	CO	ASN D	54	49.102	71.221	39.639 39.482	1.00	249.24
	5003 5004	Ň	ILE D	55	47.341	69.785	38.403	1.00	249.24
40	5005	CA	ILE D	55	47.874	68.962 67.589	38.934	1.00	185.84
40	5006	CB	ILE D	55	48.369 48.373	66.564	37.819	1.00	185.84
	5007	CG2	ILE D	55 55	49.764	67.751	39.564	1.00	185.84 185.84
	5008	CG1	ILE D	55	50.346	66.474	40.129	1.00 1.00	249.24
45	5009	CD1 C	ILE D	55	46.742	68.738	37.416 37.750	1.00	249.24
45	5010 5011	ŏ	ILE D	55	45.735	68.117	36.205	1.00	249.05
	5012	Ň	VAL D	56	46.903	69.251 69.090	35.198	1.00	249.05
	5013	CA	VAL D	56	45.870 45.719	70.362	34.349	1.00	249.53
	5014	CB	VAL D	.:S 56	44.353	70.370	33.664	1.00	249.53
50		CG1	VAL D VAL D	56	45.886	71.589	35.230	1.00	249.53 249.05
	5016	CG2 C	VAL D	56	46.211	67.906	34.301	1.00 1.00	249.05
	5017 5018	ŏ	VAL D	56	46.980	67.034	34.704 33.094	1.00	232.44
	5019	Ň	ASN D	57	45.641	67.879 66.786	32.143	1.00	232.44
5:	5 5020	CA	ASN D	57		67.311	30.708	1.00	224.76
-	5021	CB	ASN D	57 57		67.743	30.292	1.00	224.76
	5022	CG	ASN D ASN D	57		66.989	30.437	1.00	224.76 224.76
	5023	OD1 ND2	ASN D	57		68.958	29.772		232.44
6	5024 () 5025	C	ASN D	57	47.149	66.031	32.410 31.940		232.44
O	() 5025 5026	ŏ	ASN D			66.398 64.9 6 3	33.186		180.25
	5027	N	ALA D			64.086	33.631		180.25
	5028	CA	ALA D			62.956	34.453	1.00	155.06
	5029	CB	ALA D			63.508	32.559		180.25
6	5 5030	C	ALA D			62.620	31.79		180.25 167.78
	5031	0 N	LYS C		9 50.209	64.009	32.53		167.78
	5032 5033	CA	LYS	5	9 51.224	63.558	31.58 31.01		249.69
	5034	CB	LYS [30.29		249.69
•	70 5035	CG	LYS	5	9 51.110	03.112			

	5036	CD CE	LYS D LYS D	59 ⁻ 59	51.889 50.965	67.003 68.013	29.845 29.165	1.00 1.00	249.69 249.69
	5037	NZ ·	LYS D	59	51.690	69.228	28.694	1.00 1.00	249.69 167.78
	5038 5039	C	LYS D	59	52.159	62.654	32.356 33.500	1.00	167.78
5	5040	ŏ	LYS D	59	52.494	62.936	31.727	1.00	220.31
ر	5041	Ň	PHE D	60	52.566	61.564 60.608	32.364	1.00	220.31
	5042	CA	PHE D	60	53 4	59.699	31.294	1.00	243.71
•	5043	СВ	PHE D	60	54.062 53.053	58.843	30.590	1.00	243.71
	5044	CG	PHE D PHE D	60 60	53.280	58.409	29.293	1.00	243.71
10	5045	CD1	PHE D PHE D	60	51.881	58.454	31.232	1.00	243.71
	5046	CD2 CE1	PHE D	60	52.357	57.600	28.639	1.00 1.00	243.71 243.71
	5047 5048	CE2	PHE D	60	50.954	57.647	30.589 29.287	1.00	243.71
	5049	cz	PHE D	60	51.194	57.217 61.240	33.202	1.00	220.31
15	5050	С	PHE D	60	54.571	60.671	34.207	1.00	220.31
	5051	0	PHE D	60	55.007 55.025	62.417	32.789	1.00	201.05
	5052	N	GLU D	61 61	56.101	63.125	33.487	1.00	201.05
	5053	CA	GLU D	61	56.5	64.332	32.653	1.00	249.69 249.69
20	5054	CB CG	GLU D	61	57.065	63.987	31.251	1.00 1.00	249.69
20	5055 5056	CD	GLU D	61	56.045	63.244	30. 38 5 30. 24 5	1.00	249.69
	5057	OE1	GLU D	61	54.897	63.728	29.835	1.00	249.69
	5058	OE2	GLU D	61	56.395	62.176 63.588	34.884	1.00	201.05
	5059	С	GLU D	61	55.671	63.803	35.757	1.00	201.05
25	5060	0	GLU D	61 62	56.512 54.359	63.735	35.086	1.00	185.73
	5061	N	ASP D ASP D	62	53.815	64.165	36.371	1.00	185.73
	5062	CA CB	ASP D	62	52.334	64.502	36.245	1.00	180.28 180.28
	5063	CG	ASP D	62	52.063	65.480	35.132	1.00 1.00	180.28
30	5064 5065	OD1	ASP D	62	52.924	66.360	34.882 34.514	1.00	180.28
50	5066	OD2	ASP D	62	50.985	65.379 63.078	37.414	1.00	185.73
	5067	С	ASP D	62	53.982 53.979	63.353	38.606	1.00	185.73
	5068	0	ASP D	62 63	54.106	61.837	36. 96 0	1.00	159.27
~ ~	5069	N	SER D SER D	63	54.292	60.711	37.864	1.00	159.27
35	5070	CA CB	SER D	63	54.380	59.390	37.086	1.00 1.00	168.15 168.15
	5071 5072	OG OG	SER D	63	53.226	59.160	36. 3 18 38.595	1.00	159.27
	5072	č	SER D	63	55.608	60.949	37.968	1.00	159.27
	5074	ŏ	SER D	63	56.640	61.192 60.889	39.918	1.00	167.46
40	5075	N	GLY D	64	55.584 56.818	61.106	40.647	1.00	167.46
	5076	CA	GLY D GLY D	64 64	56.687	61.299	42.144	1.00	167.46
	5077	C	GLY D GLY D	64	55.643	61.035	42.741	1.00	167.46 249.05
	5078	O N	GLU D	65	57.772	61.788	42.737	1.00 1.00	249.05 249.05
45	5079 5080	ĞA	GLU D	65	57.882	62.037	44.170 44.640	1.00	248.88
-43	5081	CB	GLU D	65	59.223	61.476	46.061	1.00	248.88
	5082	CG	GLU D	65	59.604	61.791 61.571	46.298	1.00	248.88
	5083	CD	GLU D	65	61.083 61.892	62.265	45.646	1.00	248.88
	5084	OE1	GLU D	65 65	61.439	60.704	47.125	1.00	248.88
50	5085	OE2	GLU D	65	57.794	63.533	44.486	1.00	249.05 249.05
	5086	C	GLU D	65	58.598	64.318	43.989	1.00 1.00	212.16
	5087 5088	Ň	TYR D	66	56.828	63.924	45.319 45.686	1.00	212.16
	5089	CA	TYR D	66		65.335 65.835	45.288	1.00	195.47
5:	5 5090	CB	TYR D	66		65.854	43.813	1.00	195.47
	5091	CG	TYR D	66		64.683	43.131	1.00	195.47
	5092	CD1	TYR D	66 66		64.715	41.795		195.47
	5093	CE1 CD2	TYR D TYR D			67.060	43.118		195.47 195.47
6	5094	CE2	TYR D			67.105	41.789		195.47
6	() 5095 5096	CZ	TYR D			65.932	41.131 39.822		195.47
	5097	он	TYR D	60		65.982 65.817	47.183		212.16
	5098	С	TYR D			65.617 64.694	47.993		212.16
	5099	0	TYR D) 6		66.906	47.534	1.00	190.15
6	5 5100	N	LYS		·	67.355	48.926		190.15
	5101	CA	LYS C	_		66.886	49,512		181.22 181.22
	5102	CB CG	LYS			67.251	48.669		181.22
	5103 5104	CD	LYS		7 60.788		49.285 48.285		181.22
•	70 5105	ČE	LYS	D 6	7 61.948	66.688	40,40		
,	, , , , , , ,				•				

i !

	5106	NZ	LYS D	67-	63.216	66.167	48.871	1.00	101.00
	5107	C	LYS D	67	56.878	68.876	49.119	1.00 1.00	181.22 190.15
	5108	Ō	LYS D	67	57.155	69.660	48.209	1.00	190.15
_	5109	N	CYS D	68	56.473	69.282	50.320	1.00	199.06
5	5110	ÇA	CYS D	68	56.346	70.695	50.654	1.00	199.06
	5111	C	CYS D	68	57.039	71.004	51.975	1.00	199.06
	5112 5113	O CB	CYS D	68	57.153	70.155	52.861	1.00	199.06
	5114	SG	CYS D	68 68	54.871 53.830	71.135 70.461	50.708 52.050	1.00	219.86
10	5115	Ň	GLN D	69	57.505	72.240	52.083	1.00 1.00	219.86
	5116	CA	GLN D	69	58.212	72.728	53.257	1.00	249.17 249.17
	5117	CB	GLN D	69	59.714	72.495	53.072	1.00	249.69
	5118	CG	GLN D	69	60.606	73.364	53.942	1.00	249.69
1.5	5119	CD	GLN D	69	62.082	73.199	53.613	1.00	249.69
1.	5120 5121	OE1 NE2	GLN D GLN D	69 60	62.491	73.322	52.452	1.00	249.69
	5122	C	GLN D	69 69	62.892 57.925	72.925 74.222	54. 63 4 53.407	1.00 1.00	249.69
	5123	ŏ	GLN D	69	57.726	74.927	52.418	1.00	249.17 249.17
	5124	N	HIS D	70	57.896	74.706	54.642	1.00	249.69
20	5125	CA	HIS D	70	57.642	76.122	54.874	1.00	249.69
	5126	CB	HIS D	70	56.693	76.309	56.060	1.00	249.61
	5127 5128	CD2	HIS D	70 70	55.290 54.464	75.881	55.773	1.00	249.61
	5129	ND1	HIS D	70 70	54.583	75.035 76.348	56.426 54.683	1.00	249.61
25	5130	CE1	HIS D	70	53.382	75.805	54.680	1.00 1.00	249.61 249.61
	5131	NE2	HIS D	70	53.280	75.003	55.727	1.00	249.61
	5132	С	HIS D	70	58.936	76.887	55.115	1.00	249.69
	5133	0	HIS D	70	60.031	76.352	54.920	1.00	249.69
30	5134	N	GLN D	71	58.803	78.140	55.540	1.00	249.69
50	5135 5136	CA CB	GLN D GLN D	71 71	59.955 59.459	79.008	55.802	1.00	249.69
	5137	CG	GLN D	71 71	59.459 60.461	80.374 81.539	56.307 56.197	1.00 1.00	249.69
	5138	CD	GLN D	71	60.863	81.861	54.754	1.00	249.69 249.69
~~	5139	OE1	GLN D	71	60.016	81.976	53.858	1.00	249.69
35	5140	NE2	GLN D	71	62.163	82.021	54.530	1.00	249.69
	5141	C	GLN D	71	60.929	78.392	56.816	1.00	249.69
	5142 5143	0 N	GLN D	71 72	62.143 60.389	78.352 77.905	56.581	1.00	249.69
	5144	CA	GLN D	72	61.203	77.301	57.932 58.984	1.00 1.00	249.69 249.69
40	5145	CB	GLN D	72	61.267	78.257	60.181	1.00	249.69 247.95
	5146	CG	GLN D	72	62.117	77.792	61.354	1.00	247.95
	5147	CD	GLN D	72	61.994	78.719	62.551	1.00	247.95
	5148	OE1	GLN D	72	62.253	79.917	62.449	1.00	247.95
45	5149 5150	NE2 C	GLN D	72 72	61.591	78.168 75.047	63.693	1.00	247.95
	5151	ŏ	GLN D	72 72	60.624 60.335	75.947 75.721	59.409 60.584	1.00 1.00	249.69
	5152	Ň	VAL D	73	60.449	75.052	58.443	1.00	249.69 248.81
	5153	CA	VAL D	73	59.911	73.726	58.720	1.00	248.81
50	5154	CB	VAL D	73	58.396	73.640	58.398	1.00	224.12
50	5155	CG1	VAL D	73	57.822	72.365	58.991	1.00	224.12
	5156 5157	CG2 C	VAL D	73 73	57.664	74.863	58.936	1.00	224.12
	5158	ŏ	VAL D	73 73	60.641	72.704 72.085	57.858 58.717	1.00	248.81
	5159	Ň	ASN D	74	60.869	72.985 71.519	56.717 58.404	1.00 1.00	248.81 237.91
55	5160	CA	ASN D	74	61.552	70.475	57.660	1.00	237.91
	5161	CB	ASN D	74	62.098	69.419	58.631	1.00	218.21
	5162	CG	ASN D	74	63.003	70.022	59. 699	1.00	218.21
	5163 5164	OD1 ND2	ASN D	74	63.818	70.893	59.398	1.00	218.21
60	5165	C	ASN D	74 74	62.865 60.595	69.553	60.940	1.00	218.21
	5166	ŏ	ASN D	74	59.477	69.846 69.450	56.635 56.973	1.00 1.00	237.91 237.91
	5167	N	GLU D	75	61.042	69.772	55.381	1.00	249.69
	5168	CA	GLU D	75	60.252	69.219	54.276	1.00	249.69
65	5169	CB	GLU D	75	61.161	68.971	53.065	1.00	244.63
O)	5170 5171	CG	GLU D	75 75	62.563	68.479	53.417	1.00	244.63
	5171 5172	CD OE1	GLU D	75 75	63.503	68.477 60.500	52.223	1.00	244.63
	5173	OE2	GLU D	75 75	63.579 64.172	69.508 67.448	51.523	1.00	244.63
	5174	č	GLU D	75	59.463	67.954	51.989 54.609	1.00 1.00	244.63 249.69
70	5175	0	GLU D	75	59.947	67.066	55.313	1.00	249.69

					50.044	67.886	54.080	1.00	245.54
	5176	N		76 ·	58.244 57.338	66.759	54.313	1.00	245.54
	5177	CA		76	55.952	67.070	53.739	1.00	192.35
	5178	CB		76 76	55.961	66.977	52.328	1.00	192.35
	5179	OG		76 76	57.811	65.437	53.721	1.00	245.54
5	5180	С	SER D	76 76	58.617	65.413	52.791	1.00	245.54
_	5181	0	SER D	76	57.289	64.340	54.268	1.00	239.60
	5182	N.	GLU D	77 77	57.628	63.013	53.788	1.00	239.60
	5183	CA	GLU D GLU D	77	56.972	61.938	54.663	1.00	249.69
	5184	CB	GLU D	77	57.497	61.895	56.089	1.00	249.69
10	5185	CG	GLU D	77	58.969	61.533	56.157	1.00	249.69
	5186	CD	GLU D	77	59.621	61.453	55.090	1.00	249.69
	5187	OE1	GLU D	77	59.476	61.333	57.282	1.00	249.69
	5188	OE2 C	GLU D	77	57.106	62.902	52.366	1.00	239.60 239.60
1.5	5189	Ö	GLU D	77	55.898	62.905	52.139	1.00 1.00	190.36
15	5190	N	PRO D	78	58.019	62.800	51.386	1.00	231.46
	5191	CD	PRO D	78	59.457	62.543	51.572 49. 96 9	1.00	190.36
	5192	CA	PRO D	78	57.642	62.695	49.320	1.00	231.46
	5193 5194	CB	PRO D	78	58.919	62.159	50.179	1.00	231.46
20	5195	ĊĠ	PRO D	78	60.002	62.732	49.731	1.00	190.36
20	5196	C	PRO D	78	56.456	61.764	50.553	1.00	190.36
	5197	ō	PRO D	78	56.163	60.897	48.620	1.00	182.77
	5198	N	VAL D	79	55.760	61.969 61.112	48.261	1.00	182.77
	5199	CA	VAL D	79	54.639	61.804	48.426	1.00	114.23
25	5200	СВ	VAL D	79	53.272	60.961	47.770	1.00	114.23
20	5201	CG1	VAL D	79	52.173	61.977	49.909	1.00	114.23
	5202	CG2	VAL D	79	52.957	60.799	46.800	1.00	182.77
	5203	С	VAL D	79	54.845 55.292	61.663	46.043	1.00	182.77
	5204	0	VAL D	79	55.292 54. 53 8	59.570	46.397	1.00	172.05
30	5205	N	TYR D	80 80	54.726	59.204	45.004	1.00	172.05
	5206	CA	TYR D	80	55.475	57.870	44.888	1.00	249.30
	5207	CB ·	TYR D TYR D	80	56.087	57.651	43.518	1.00	249.30
	5208	CG	TYR D	80	57.327	58.197	43.191	1.00	249.30
~~	5209	CD1 CE1	TYR D	80	57.868	58.042	41.917	1.00	249.30 249.30
35	5210	CD2	TYR D	80	55.403	56.940	42.531	1.00 1.00	249.30
	5211	CE2	TYR D	80	55.937	56.780	41.254	1.00	249.30
	5212 5213	CZ	TYR D	80	57.167	57.335	40.956 39. 69 6	1.00	249.30
	5213 5214	OH	TYR D	80	57.689	57.191	44.238	1.00	172.05
40	5215	Č	TYR D	80	53.407	59.120	44.701	1.00	172.05
40	5216	Õ	TYR D	80	52.419	58.550 59.702	43.054	1.00	138.80
	5217	N	LEU D	81	53.407	59.681	42.207	1.00	138.80
	5218	CA	LEU D	81	52.239	61.099	41.821	1.00	163.84
	5219	CB	LEU D	81	51.837 50.683	61.126	40.812	1.00	163.84
45	5220	CG	LEU D	81	49.462	60.512	41.463	1.00	163.84
	5221	CD1	LEU D	81 81	50.394	62.539	40.357	1.00	163.84
	5222	CD2	LEU D	81	52.560	58.907	40.932	1.00	138.80
	5223	C	LEU D	81		59.196	40.251	1.00	138.80
	5224	0	GLU D	82		57.924	40.598	1.00	140.95 140.95
50		N CA	GLU D	82		57.14 9	39.380	1.00	249.69
	5226	CB	GLU D	82		55.662	39.716	1.00	249.69
	5227	CG	GLU D	82	52.985	54.915	38.685	1.00 1.00	249.69
	5228 5229	CD	GLU D	82		53.447	39.028 40.233	1.00	249.69
5	5 5230	OE1	GLU D	82		53.118	38.088	1.00	249.69
5	5231	OE2	GLU D	82		52.623	38.415		140.95
	5232	C	GLU D	83		57.324 57.327	38.824		140.95
	5233	0	GLU D	8		57.287 57.533	37.139		204.94
	5234	N	VAL D			57.704	36.106		204.94
6	0 5235	CA	VAL D			58.985	35.282		154.41
•	5236	CB	VAL D	8		59.119	34,248		154.41
	5237	CG1	VAL D	. 8	3 49.194 3 50.333	60.203	36.207	1.00	154.41
	5238	CG2	VAL D	, 6	3 50.333 3 50.072	56.510	35.159	1.00	204.94
	5239	Ç	VAL D		3 51.125	55.962	34.781		204.94
•	55 5240	0	VAL D		34 48.858	56.137	34.75		140.70
	5241	N	PHE C		48.655	54.961	33.91		140.70
	5242	CA	PHE C		48.013	53.843	34.73		172.63 172.63
	5243	CB CB	PHE	-	84 48.828	53.387	35.90		172.63
	5244 70 5245	CD1		-	84 48.823	54.095	37.10	2 1.00	(72.00
	, 5 52-55								

			DUE D	84	49.579	52.229	35.815	1.00	172.63
	5246	CD2	PHE D PHE D	84	49.553	53.648	38.187	1.00	172.63
	5247	CE1 CE2	PHE D	84	50.310	51.776	36.892	1.00	172.63
	5248	CZ	PHE D	84	50.298	52.483	38.084	1.00	172.63
5	5249	C	PHE D	84	47.811	55.075	32.669	1.00	140.70
3	5250 5251	ŏ	PHE D	84	46.952	55.941	32.546	1.00 1.00	140.70 187.78
	5252	Ň	SER D	85	48.057	54.127	31.773 30.534	1.00	187.78
	5253	CA	SER D	85	47.318	53.999	29.322	1.00	228.86
	5254	СВ	SER D	85	48.163	54. 364 54. 223	28.141	1.00	228.86
10	5255	OG	SER D	85	47.394	52.522	30.461	1.00	187.78
	5256	С	SER D	85	46.957 47.841	51.663	30.344	1.00	187.78
	5257	0	SER D	85 86	45.657	52.235	30.551	1.00	145.83
	5258	N	ASP D ASP D	86	45.141	50.864	30.508	1.00	145.83
15	5259	CA CB	ASP D	86	45.692	50.069	31.690	1.00	155.62
15	5260 5261	CG	ASP D	86	45.997	48.650	31.328	1.00 1.00	155.62 155.62
	5262	OD1	ASP D	86	45.107	47.971	30.755 31.610	1.00	155.62
	5263	002	ASP D	86	47.133	48.214	30.580	1.00	145.83
	5264	C	ASP D	86	43.621	50.885 51.914	30.878	1.00	145.83
20	5265	0	ASP D	86	43.019	49.749	30.315	1.00	152.62
	5266	N	TRP D	87	42.997 41.544	49.688	30.387	1.00	152.62
	5267	CA	TRP D	87 87	41.038	48,369	29.817	1.00	249.69
	5268	CB	TRP D	B7	40.784	48.449	28.349	1.00	249.69
25	5269	CG CD2	TRP D	87	41.700	48.112	27.306	1.00	249.69
25	5270	CE2	TRP D	87	41.058	48. 38 5	26.079	1.00	249.69 249.69
	5271 5272	CE3	TRP D	87	43.010	47.599	27.285	1.00 1.00	249.69
	5273	CD1	TRP D	87	39.649	48.907	27.735 26.373	1.00	249.69
	5274	NE1	TRP D	87	39.807	48.868 48.164	24.845	1.00	249.69
30	5275	CZ2	TRP D	87	41.674	46.104 47.377	26.056	1.00	249.69
	5276	CZ3	TRP D	87	43.623 42.955	47.666	24.854	1.00	249.69
	5277	CH2	TRP D TRP D	87 87	41.058	49.854	31.821	1.00	152.62
	5278	C O	TRP D	87	40.220	50.708	32.092	1.00	152.62
25	5279	N	LEU D	88	41.578	49.041	32.739	1.00	136.73 136.73
35	5280 5281	CA	LEU D	88	41.190	49.161	34.137	1.00 1.00	120.19
	5282	CB	LEU D	88	40.415	47.933	34.574 33.876	1.00	120.19
	5283	CG	LEU D	88	39.068	47.722 46.521	34,481	1.00	120.19
	5284	CD1	LEU D	88	38.314	48.972	34.012	1.00	120.19
40	5285	CD2	LEU D	88	38.232 42.405	49.364	35.043	1.00	136.73
	5286	Ç	LEU D	88 88	43.486	48.794	34.806	1.00	136.73
	5287	0	LEU D	89	42,238	50.206	36.063	1.00	129.46
	5288	N CA	LEU D	89	43,315	50.483	37.021	1.00	129.46 166.27
45	5289 5290	CB	LEU D	89	43.867	51.888	36.838	1.00	166.27
45	5290 5291	CG	LEU D	89	44.935	52.257	37.864	1.00 1.00	166.27
	5292	CD1	LEU D	89	46.034	51.209	37.875 37.532	1.00	166.27
	5293	CD2	LEU D	89	45.502	53.621 50.361	38.425	1.00	129.46
	5294	С	LEU D	89	42.751 41.706	50.925	38.731	1.00	129.46
50		0	LEU D	89 9 0	43.435	49.611	39.278	1.00	149.29
	5296	N	LEU D	90	42.966	49.415	40.640	1.00	149.29
	5297	CA	LEU D	90	43.433	48.070	41.171	1.00	119.67
	5298	CB CG	LEU D	90	43.122	47.859	42.640	1.00	119.67 119.67
55	5299 5300	CD1	LEU D	90	41.612	47.911	42.843	1.00 1.00	119.67
33	5301	CD2	LEU D	90		46.531	43.108 41.543	1.00	149.29
	5302	C	LEU D	90		50.508	41.785	1.00	149.29
	5303	0	LEU D	90		50.591 51.336	42.059	1.00	104.53
	5304	N	GLN D	91		52.439	42.946	1.00	104.53
60		CA	GLN D	91 91		53.716	42.566	1.00	160.34
	5306	CB	GLN D			54.188	41.147	1.00	160.34
	5307	CG	GLN D GLN D			55.470	40.843	1.00	160.34
	5308	CD OE1	GLN D			55.541	40.995	1.00	160.34 160.34
6:	5309 5 5310	NE2	GLN D		42.485	56.493	40.412	1.00 1.00	104.53
U.	5311	Ċ	GLN D	9.		52.156	44.424 44.823		104.53
	5312	ŏ	GLN D			51.645 52.506	45.227		107.84
	5313	N	ALA D			52.506 52.285	46.657		107.84
	5314	CA	ALA D			52.285 51.297	47.102		189.20
7	0 5315	CB	ALA D	9:	Z 44./31				

				o2.	43.850	53.594	47.399	1.00	107.84
	316	Ç	ALA D ALA D		44.683	54.436	46.987	1.00	107.84
	317	0	SER D		43.062	53.754	48.477	1.00	115.75
	318	N .	SER D		43.108	54.947	49.319	1.00	115.75
_ 50	319	CA .	SER D	93	42.212	54.756	50.553	1.00	115.29 115.29
	320	CB OG	SER D	93	42.503	53.560	51.271	1.00 1.00	115.25
	321 322	C	SER D	93	44.559	55.177	49.730 49.371	1.00	115.75
	323	ŏ	SER D	93	45.176	56.193	50.476	1.00	146.78
	324	N	ALA D	94	45.094	54.214 54.242	50.924	1.00	146.78
	325	CA	ALA D	94	46.481 46.552	54.536	52.412	1.00	207.94
5	326	CB	ALA D	94 94	46.992	52.846	50.626	1.00	146.78
	327	C	ALA D ALA D	94	46.194	51.905	50.566	1.00	146.78
	328	0	GLU D	95	48.300	52.699	50.426	1.00	134.86 134.86
5 م	329	N CA	GLU D	95	48.844	51.383	50.125	1.00 1.00	220.03
	5330 5331	CB	GLU D	95	49.967	51.498	49.101 47.768	1.00	220.03
	5332	CG	GLU D	95	49.489	52.026	46.687	1.00	220.03
	5333	CD	GLU D	95	50.535	51.898 52.341	45.547	1.00	220.03
	5334	OE1	GLU D	95 05	50.271	51.351	46.970	1.00	220.03
20	5335	OE2	GLU D	95 95	51.621 49.335	50.662	51.376	1.00	134.86
:	5336	Ç	GLU D GLU D	95	49.412	49.423	51.408	1.00	134.86
	5337	0	VAL D	96	49.655	51.439	52.407	1.00	128.32 128.32
	5338	N CA	VAL D	96	50.122	50.876	53.668	1.00	128.32
25	5339	CB	VAL D	96	51.561	51.292	53.949 55.003	1.00 1.00	128.30
23	5340 5341	CG1	VAL D	96	52.157	50.377	52.675	1.00	128.30
	5342	CG2	VAL D	96	52.372	51.260 51.383	54.816	1.00	128.32
	5343	С	VAL D	96	49.242	52.588	54.932	1.00	128.32
	5344	0	VAL D	96 97	49.010 48.775	50.480	55.678	1.00	152.31
30	5345	N	VAL D VAL D	97	47.890	50.898	56.756	1.00	152.31
	5346	CA CB	VAL D	97	46.438	50.575	56.406	1.00	113.44 113.44
	5347	CG1	VAL D	97	45.533	51.442	57.216	1.00 1.00	113.44
	5348 5349	CG2	VAL D	97	46.185	50.774	54.941 58.152	1.00	152.31
35	5350	Č	VAL D	97	48.135	50.330 49.193	58.305	1.00	152.31
55	5351	0	VAL D	97	48.616	51.133	59.160	1.00	133.53
	5352	N	MET D	98 98	47.765 47.880	50.784	60.590	1.00	133.53
	535 3	CA	MET D	98	47.936	52.058	61.440	1.00	228.89
40	5354	CB CG	MET D	98	49.145	52. 9 51	61.220	1.00	228.89 228.89
40	5355	SD	MET D	98	50.627	52.296	62.005	1.00 1.00	228.89
	5356 5357	CE	MET D	98	50.300	52.679	63.720 61.010	1.00	133.53
	5358	Č	MET D	98	46.651	49.985 50.470	60.868	1.00	133.53
	5359	0	MET D	98	45.535	48.786	61.547	1.00	198.14
45	5360	N	GLU D	99	46.849 45.726	47.954	61.963	1.00	198.14
	5361	CA	GLU D	99 99	46.179	46.922	63.001	1.00	249.68
	5362	CB	GLU D	99	45.303	45.675	63.049	1.00	249.68 249.68
	5363	CG CD	GLU	99	45.586	44.809	64.259	1.00 1.00	249.68
50	5364 5365	OE1	GLU D	99	48.770	44.698	64.645 64.816	1.00	249.68
30	5366	DE2	GLU D	99	44.627	44. 23 3 48.812	62.563	1.00	198.14
	5367	C	GLU D	99		49.583	63.489	1.00	198.14
	5368	0	GLU D	99		48.692	62.031	1.00	166.74
	5369	N.	GLY D	10 10		49.467	62.569		166.74
55	5370	ÇA	GLY D	10		50.625	61.718		166.74 166.74
	5371	င 0	GLY D			51.053	61.861		134.36
	5372 5373	Ň	GLN D			51.133	60.842		134.36
	5374	ĞA	GLN D	10		52.250	59.961 59.372		207.44
60	5375	СВ	GLN D			52.882 53.630	60.387		207.44
00	5376	CG	GLN D		01 44.392	54.494	61.269		207.44
	5377	CD	GLN D		01 43.524 01 42.774	53.987	62.103	3 1.00	207.44
•	5378	OE1	GLN D		01 42.774 01 43.607	55.807	61.083		207.44
,	5379	NE2	GLN D		01 41.345	51.862	58.84		134.36 134.36
65		C	GLN C		01 41.004	50.693	58.67		115.73
	5381 5382	Ň	PRO		02 40.894	52.871	58.05		176.17
	5382 5383	CD	PRO I) 1	02 40.996	54.307 50.560	58.28 56.94	-	115.73
	5384	CA	PRO	-	02 39.973	52.569 53.843	56.89		176.17
70		СВ	PRO I	ו כ	02 39.138		55.35		

	5386	CG	PRO D	102	40.181	54.884	57.136	1.00	176,17
	5387	C	PRO D	102	40.678	52.280	55.630	1.00	115.73
	5388	0	PRO D	102	41.771	52.810	55.342	1.00	115.73
5	5389	N	LEU D	103 103	40.042 40.610	51.439 51.062	54.818 53.547	1.00 1.00	118.65
)	5390 5391	CA CB	LEU D	103	41.185	49.671	53.652	1.00	118.65 120.76
	5392	CG	LEU D	103	42.003	49.394	52.400	1.00	120.76
	5393	CD1	LEU D	103	43.228	50.310	52.430	1.00	120.76
	5394	CD2	LEU D	103	42.399	47.938	52.323	1.00	120.76
10	5395	C	LEU D	103	39.597	51.065 50.389	52.413 52.508	1.00	118.65
	5396 5397	0 N	LEU D PHE D	103 104	38.575 39.875	51.798	51. 33 2	1.00 1.00	118.65 129.85
	5398	CA	PHE D	104	38.955	51.830	50.187	1.00	129.85
	5399	СВ	PHE D	104	38.327	53.199	50.024	1.00	234.23
15	5400	CG	PHE D	104	37.655	53.699	51.249	1.00	234.23
	5401	CD1	PHE D	104	38.402	54.218	52.300	1.00	234.23
	5402 5403	CD2 CE1	PHE D PHE D	104 104	36.273 37.779	53.651 54.688	51.365 53.457	1.00 1.00	234.23 234.23
	5404	CE2	PHE D	104	35.638	54.116	52.517	1.00	234.23
20	5405	CZ	PHE D	104	36.393	54.637	53.567	1.00	234.23
	5406	С	PHE D	104	39.651	51.480	48.881	1.00	129.85
	5407	0	PHE D	104	40.632	52.139	48.499	1.00	129.85
	5408	N	LEU D	105	39.152	50.446 50.039	48.198 46.914	1.00 1.00	126.08 126.08
25	5409 5410	CA CB	LEU D	105 105	39.725 40.031	48.548	46.910	1.00	130.08
23	5411	CG	LEU D	105	41.013	48.106	47.993	1.00	130.08
	5412	CD1	LEU D	105	41.358	46.640	47.803	1.00	130.08
	5413	CD2	LEU D	105	42.266	48.976	47.919	1.00	130.08
20	5414	Ç	LEU D	105	38.719	50.360	45.832	1.00	126.08
30	5415	0	LEU D ARG D	105 106	37.510 39.203	50.328 50.658	46.061 44.641	1.00 1.00	126.08 133.86
	5416 5417	N CA	ARG D	106	38.288	51.013	43.581	1.00	133.86
	5418	CB	ARG D	106	38.213	52.537	43.522	1.00	170.25
	5419	CG	ARG D	106	37.267	53.090	42.509	1.00	170.25
35	5420	CD	ARG D	106	37.416	54.594	42.401	1.00	170.25
	5421	NE OZ	ARG D	106	36.634 36.946	55.086 56.155	41.272 40.553	1.00 1.00	170.25 170.25
	5422 5423	CZ NH1	ARG D ARG D	106 106	38.031	56.855	40.841	1.00	170.25
	5424	NH2	ARG D	106	36.181	56.503	39.529	1.00	170.25
40	5425	C	ARG D	106	38.732	50.439	42.239	1.00	133.86
	5426	0	ARG D	106	39.882	50.624	41.824	1.00	133.86
	5427	N OA	CYS D	107	37.833 38.144	49.718 49.158	41.572 40.256	1.00 1.00	163.35 163.35
	5428 5429	CA C	CYS D CYS D	107 107	37.800	50.290	39.316	1.00	163.35
45	5430	ŏ	CYS D	107	36.621	50.528	39.043	1.00	163.35
	5431	СВ	CYS D	107	37.250	47.960	39.954	1.00	164.16
	5432	SG	CYS D	107	37.777	46.964	38.529	1.00	164.16
	5433	N	HIS D	108	38.824	50.991	38.834 37.962	1.00 1.00	196.08
50	5434 5435	CA CB	HIS D HIS D	108 108	38.626 39.641	52.153 53.252	38.313	1.00	196.08 199.66
50	5436	CG	HIS D	108	39.354	54.579	37.678	1.00	199.66
	5437	CD2	HIS D	108	40.151	55.424	36.978	1.00	199.66
	5438	ND1	HIS D	108	38.135	55.214	37.796	1.00	199.66
<i>e</i>	5439	CE1	HIS D	108	38.197	56.390	37.202	1.00	199.66
55	5440	NE2	HIS D HIS D	108 108	39.411 38.691	56.543 51.885	36.699 36.473	1.00 1.00	199.66 196.08
	5441 5442	C O	HIS D	108	39.670	51.330	35.865	1.00	196.08
	5443	Ň	GLY D	109	37.636	52.310	35.785	1.00	171.21
	5444	CA	GLY D	109	37.566	52.139	34.354	1.00	171.21
60	5445	Ç	GLY D	109	38.291	53.283	33.690	1.00	171.21
	5446	0	GLY D	109	38.608	54.272 63.141	34.344	1.00	171 <i>.</i> 21 191.90
	5447 5448	N CA	TRP D	110 110	38.566 39.258	53.141 54.181	32.395 31.637	1.00 1.00	191.90
	5449	CB	TRP D	110	40.029	53.562	30.453	1.00	203.94
65	5450	ÇĞ	TRP D	110	40.592	54.575	29.502	1.00	203.94
	5451	CD2	TRP D	110	41.946	55.053	29.444	1.00	203.94
	5452	CE2	TRP D	110	41.995	56.035	28.434	1.00	203.94
	5453	CE3	TRP D	110 110	43.117	54.754 55.256	30.151 28.549	1.00 1.00	203.94 203.94
70	5454 5455	CD1 NE1	TRP D	110	39.904 40.740	56.136	26.549 27.907	1.00	203.94
. •	~~								

					40.470	56.718	28.110	1.00	203.94
	5456	CZ2	TRP D	110	43.173 44.291	55.439	29.823	1.00	203.94
	5457	CZ3	TRP D	110 110	44.305	56.406	28.809	1.00	203.94
	5458	CH2	TRP D	110	38.245	55.224	31.155	1.00 1.00	191.90 191.90
_	5459	C	TRP D	110	37.070	54.922	30.950 30.987	1.00	162.83
5	5460	0 N	ARG D	111	38.715	56.454	30.568	1.00	162.83
	5461 5462	CA	ARG D	111	37.866	57.551 57.418	29.098	1.00	249.69
	5463	CB	ARG D	111	37.487	58.111	28.158	1.00	249.69
	5464	CG	ARG D	111	38.456 37.865	58.254	26.769	1.00	249.69
10	5465	CD	ARG D	111 111	38.203	59.544	26.175	1.00	249.69 249.69
	5466	NE	ARG D ARG D	111	37.865	60.717	26.705	1.00 1.00	249.69
	5467	CZ	ARG D	111	37.178	60.769	27.840 26.098	1.00	249.69
	5468	NH1 NH2	ARG D	111	38.209	61.844	31.415	1.00	162.83
15	5469 5470	C	ARG D	111	36.612	57.597 58.005	30.954	1.00	162.83
13	5470 5471	ŏ	ARG D	111	35.552 36.744	57.175	32.663	1.00	190.45
	5472	N	ASN D	112	35.632	57.162	33.595	1.00	190.45
	5473	CA	ASN D ASN D	112 112	35.305	53.593	34.044	1.00	228.54 228.54
	5474	CB	ASN D	112	34.442	58.632	35.296 35.701	1.00 1.00	228.54
20	5475	CG OD1	ASN D	112	33.860	57.622	35.701	1.00	228.54
	5476	ND2	ASN D	112	34.352	59.805 56.509	32.982	1.00	190.45
	5477 5478	C	ASN D	112	34.389	56.879	33.318	1.00	190.45
	5479	ō	ASN D	112	33.263 34.582	55.549	32.078	1.00	238.93
25	5480	N	TRP D	113 113	33.437	54.868	31.475	1.00	238.93
	5481	CA	TRP D	113	33.872	53.936	30.353	1.00	249.51 249.51
	5482	CB	TRP D	113		54.608	29.061	1.00 1.00	249.51
	5483	CG CD2	TRP D	113		54,251	28.071 26.973	1.00	249.51
20	5484	CE2	TRP D	113	34.860	55.110	28.013	1.00	249.51
30	5485 5486	CE3	TRP D	113		53.296 55.626	28.538	1.00	249.51
	5487	CD1	TRP D	113		55.940	27.283	1.00	249.51
	5488	NE1	TRP D	113 113		55.038	25.816	1.00	249.51 249.51
	5489	CZ2	TRP D	113		53.222	26.864	1.00 1.00	249.51
35		CZ3	TRP D	113		54.088	25.779 32.530	1.00	238.93
	5491	CH2 C	TRP D	113		54.037	33.719	1.00	238.93
	5492 5493	ŏ	TRP D	113		54.178 53.167	32.096	1.00	249.69
	5494	Ň	ASP D	11		52.312	33.034	1.00	249.69
40		CA	ASP D	11		52.451	32.843	1.00	249.69
7.	5496	CB	ASP D	11 11	·	53.672	33.560		249.69 249.69
	5497	CG	ASP D ASP D	11		53.780	34.798		249.69
	5498	OD1 OD2	ASP D	11		54.522	32.887 32.895		249.69
4.	5499	C	ASP D	11	4 31.538	50.845	31.778		249.69
4:	5 5500 5501	ŏ	ASP D		14 31.612	50.312 50.203	34.032		198.18
	5502	Ň	VAL D		15 31.825 15 32.232	48.800	34.043	1.00	198.18
	5503	CA	VAL D		15 32.232 15 33.535	48.596	34.828		157.60 157.60
	5504	СВ	VAL D		15 34.102	47.220	34.521		157.60
5	0 5505	CG1 CG2	VAL D		15 34.539	49.673	34.470		198.18
	5506	C	VAL D		15 31.149	47.938	34.68 35.68		198.18
	5507 5508	ŏ	VAL D	1	15 30.530	48.329 46.764	34.09		134.91
	5509	N	TYR D) 1	16 30.933	45.824	34.57		134.91
. 4	55 5510	CA	TYR D]	16 29.922 16 28.849	45.620	33.50		249.45
•	5511	СВ	TYR		16	40.074	33.19		249.45 249.45
	5512	CG	TYR (116 28.381	47.679	32.09		249.45
	5513	CD1 CE1	TYR		116 27.673	48.861	31.84 34.03		249.45
	5514 60 5515	CD2			116 27.023		33.78		249.45
,	5516	CE2	TYR	D	116 26.312		32.6		249.45
	5517	CZ	TYR	D	116 26.638 116 25.933		32.4	62 1.00	249.45
	5518	ÓН	TYR		116 25.933 116 30.536	44.400	34.9		134.91 134.91
	5519	C	TYR		116 31.70	6 44.205	34.6		179.36
	65 5520	0	TYR LYS	ŏ	117 29.73	9 43.615	35.6		
	5521	N CA	LYS		117 30.18		36.0 34.8	• • • • • • • • • • • • • • • • • • • •	242.00
	5522 5523	CB	LYS	D	117 30.27		34.4		249.69
	5524	CG		D	117 28.96	~~~~	33.6		
	70 5525	CD	LYS	D	117 29.20				

	5526	CE NZ	LYS D	117 117	30.074 30.356	38.376 37.108	34.424 33.677 36.769	1.00 1.00 1.00	249.69 249.69 179.36
	5527 5529	C	LYS D	117	31.531	42.338	36.425	1.00	179.36
	5528 5529	ŏ	LYS D	117	32.463	41.608 43.189	37.783	1.00	143.78
5	5530	N	VAL D	118	31.611 32.837	43.356	38.531	1.00	143.78
9	5531	CA	VAL D	118 118	32.928	44.783	39.076	1.00	119.69
	5532	CB	VAL D VAL D	118	33.829	44.851	40.289	1.00	119.69
	5533	CG1	VAL D VAL D	118	33.481	45.684	37.995	1.00	119.69 143.78
	5534	CG2	VAL D	118	33.071	42.366	39.664 40.411	1.00 1.00	143.78
10	5535	C	VAL D	118	32.142	41.998	39.775	1.00	115.37
	5536 5537	Ň	ILE D	119	34.341	41.948 41.005	40.796	1.00	115.37
	5538	CA	ILE D	119	34.809 34.981	39.618	40.220	1.00	109.20
	5539	CB	ILE D	119 119	35.367	38.649	41.306	1.00	109.20
15	5540	CG2	ILE D ILE D	119	33.691	39.187	39.545	1.00	109.20 109.20
	5541	CG1	ILE D	119	33.917	38.153	38.481	1.00 1.00	115.37
	5542	CD1 C	ILE D	119	36.184	41.446	41.260 40.429	1.00	115.37
	5543 5544	ŏ	ILE D	119	37.068		42.573	1.00	120.82
20	5545	Ň	TYR D	120	36.364		43.089	1.00	120.82
20	5546	CA	TYR D	120	37.664 37.537		44.308	1.00	123.48
	5547	СВ	TYR D	120 120	37.016		44.008	1.00	123.48
	5548	CG	TYR D TYR D	120	35.652		43.958	1.00	123.48 123.48
	5549	CD1	TYR D	120	35.154	45.696	43.664	1.00 1.00	123.48
25	5550	CE1 CD2	TYR D	120	37.889		43.758 43.464	1.00	123.48
	5551	CE2	TYR D	120	37.40		43.419	1.00	123.48
	5552 5553	cz	TYR D	120	36.03		43.132	1.00	123.48
	5554	OH	TYR D	120	35.55 38.34		43.500	1.00	120.82
30	5555	C	TYR D	120 120			43.881	1.00	120.82
-	5556	0	TYR D TYR D	121			43.420	1.00	108.96 108.96
	5557	N	TYR D	121		2 39.364	43.803	1.00 1.00	127.51
	5558	CA CB	TYR D	121		7 38.672	42.579 41.600	1.00	127.51
25	5559	CG	TYR D	121			40.928	1.00	127.51
35	5560 5561	CD1	TYR D	121			39.947	1.00	127.51
	5562	CE1	TYR D	121		~	41.277	1.00	127.51
	5563	CD2	TYR D	121 121	•		40.302	1.00	127.51 127.51
	5564	CE2	TYR D	12			39.635	1.00	127.51
40	5565	CZ	TYR D	12	•	66 38.374	38.642	1.00 1.00	108.96
	5566	C OH	TYR D	12	1 41.5	40.004	44.755 44.539	1.00	108.96
	5567 5568	ŏ	TYR D	12			45.807	1.00	150.86
	5569	Ň	LYS D	12			46.762	1.00	150.86
45		CA	LYS D	12 12			48.145	1.00	185.53
	5571	CB	LYS D	12			49.176	1.00	185.53 185.53
	5572	CG	LYS D LYS D	12		724 39.656	50.576		185.53
	5573	CD CE	LYS D	12		39.686	51.615 52.970		185.53
50	5574	NZ	LYS D		22 43.		46.834		150.86
3() 5575 5576	c	LYS D		22 43.4		47,210		150.86
	5577	Ö	LYS D		22 42. ⁹ 23 44.		46.463	1.00	129.20
	5578	N	ASP D			601 36.577	46.485		129.20 160.45
_	5579	CA	ASP D			857 36.104	47.924		160.45
5		CB CG	ASP D		23 46.	852 36.986	48.66° 48.09		160.45
	5581	OD1	ASP D			927 37.268	40.00		160.45
	5582 5583	OD2	ASP D	1		.572 37.390 .999 35.441			129.20
	5584	C	ASP D			,999 35.441 .855 34.331	46.20	5 1.00	129.20
6	0 5585	0	ASP D			.643 35.729	44.43		131.93
_	5586	N.	GLY D			.085 34.715	43.54		131.93 131.93
	5587	CA	GLY C			.682 34.206			131.93
	5588	CO	GLY C	-	124 42	2.137 33.416			141.53
4	5589 55 5590	Ň	GLU [)		2.093 34.656	4		141.53
(5591	ĊA	GLU ()		0.751 34.229 0.682 34.03		1.00	249.69
	5592	CB	GLU I	-		0.682 34.03 1.469 32.84	·	72 1.00	249.69
	5593	CG	GLU !			0.788 31.51	2 47.0		249.69 249.69
	5594	CD	GLU GLU			9.664 31.29		71 1.00	249.08
	70 5595	OE1	GLO						

		050	GLU D	125	11.373	30.682	46.346	1.00	249.69
	5596	OE2 C	GLU D		39.673	35.224	44.897	1.00	141.53
	5597 5598	ŏ	GLU D		39.903	36.441	44.907	1.00	141.53
	5599	Ň	ALA D	126	38.503	34.707	44.520	1.00	148.59
5	5600	CA	ALA D		37.393	35.570	44.136	1.00	148.59
•	5601	ÇB	ALA D		38.274	34.743	43.560 45.453	1.00 1.00	144.26 148.59
	5602	С	ALA D		36.961	36.205 35.516	45.453 46.481	1.00	148.59
	5603	0	ALA D		36.909 36.652	37.501	45.448	1.00	169.46
	5604	N	LEU D		36.632 36.274	38.153	46.700	1.00	169.46
10	5605	CA	LEU D		37.294	39.224	47.040	1.00	146.34
	5606 5607	CB CG	LEU D		37.368	39.389	48.547	1.00	146.34
	5608	CD1	LEU D		37.671	38.030	49.183	1.00	146.34
	5609	CD2	LEU D		38.440	40.394	48.897	1.00	146.34
15	5610	C	LEU D		34.880	38.750	46.796	1.00	169.46
	5611	0	LEU D		34.081	38.350	47.640 45.957	1.00 1.00	169.46 129.34
	5612	N	LYS D	128	34.609	39.738 40.371	45.930	1.00	129.34
	5613	CA	LYS D	128	33.302	41.784	46.505	1.00	216.92
	5614	CB	LYS D	128 128	33.390 33.863	41.849	47.952	1.00	216.92
20	5615	CG	LYS D LYS D	128	32.806	41.345	48.935	1.00	216.92
	5616	CD CE	LYS D	128	33.279	41.519	50.376	1.00	216.92
	5617 5618	NZ	LYS D	128	32.194	41.270	51. 36 6	1.00	216.92
	5619	C	LYS D	128	32.834	40.419	44.475	1.00	129.34
25	5620	ŏ	LYS D	128	33.645	40.314	43.556	1.00	129.34 159.52
	5621	N	TYR D	129	31.532	40.581	44.261 42.907	1.00 1.00	159.52
	5622	CA	TYR D	129	31.000	40.642	42.432	1.00	146.13
	5623	СВ	TYR D	129	30.682	39.239 39.234	41.246	1.00	146.13
20	5624	CG	TYR D	129 129	29.763 30.255	39.420	39.958	1.00	146.13
30	5625	CD1 CE1	TYR D	129	29.395	39.478	38.859	1.00	146.13
	5626 5627	CD2	TYR D	129	28.380	39.103	41.419	1.00	146.13
	5628	CE2	TYR D	129	27.507	39.162	40.337	1.00	146.13
	5629	CZ	TYR D	129	28.021	39.350	39.055	1.00	146.13
35	5630	OH	TYR D	129	27.158	39.406	37.976	1.00 1.00	146.13 159.52
_	5631	С	TYR D	129	29.747	41.516 41.489	42.767 43.622	1.00	159.52
	5632	0	TYR D	129	28.858 29.676	42.283	41.678	1.00	181.39
	5633	N	TRP D TRP D	130 130	28.519	43,144	41.418	1.00	181.39
40	5634 5635	CA CB	TRP D	130	28.703	44.540	42.021	1.00	248.73
40	5636	ČG	TRP D	130	29.193	44.604	43. 43 6	1.00	248.73
	5637	CD2	TRP D	130	28.426	44.935	44.598	1.00	248.73
	5638	CE2	TRP D	130	29.302	44.930	45.703	1.00 1.00	248.73 248.73
	5639	C ⊵ 3	TRP D	130	27.074	45.246	44.816 43.872	1.00	248.73
45	5640	CD1	TRP D	130	30.471 30.551	44.405 44.606	45. 22 9	1.00	248.73
	5641	NE1	TRP D	130 130	28.883	45.219	47.005	1.00	248.73
	5642	CZ2 CZ3	TRP D	130	26.651	45.532	48.11 6	1.00	248.73
	5643 5644	CH2	TRP D	130	27.555	45.511	47.192	1.00	248.73
50	5645	C	TRP D	130	28.281	43.326	39.916	1.00	181.39
50	5646	ŏ	TRP D	130	29.126	42.952	39.090	1.00	181.39
	5647	N	TYR D	131	27.129	43.907	39.576	1.00	195.20 195.20
	5648	· GA	TYR D	131	26.776	44.183	38,185 38,020	1.00	249.67
	5649	CB	TYR D	131	25.263	44.162 44.143	36.579	1.00	249.67
55	5650	CG	TYR D	131 131	24.831 24.974	42.992	35.806	1.00	249.67
	5651	CD1	TYR D TYR D	131	24.612	42.979	34.465	1.00	249.67
	5652 5653	CE1 CD2	TYR D	131	24.311	45.285	35.973	1.00	249.67
	5654	CE2	TYR D	131	23.949	45.285	34.632	1.00	249.67
60	5655	CZ	TYR D	131	24.101	44.131	33.884	1.00	249.67
•	5656	ОН	TYR D	131	23.751	44.140	32.553	1.00	249.67 195.20
	5657	С	TYR D	131	27.319	45.591	37.904	1.00 1.00	195.20
	5658	0	TYR D	131	28.458	45.748 48.814	37.468 38.131	1.00	246.45
	5659	N	GLU D	132	26.492 26.949	46.614 47.994	37.982	1.00	246.45
65	5660	CA	GLU D	132 132	25.841	48.983	38.357	1.00	249.69
	5661	CB	GLU D	132	24.774	49.219	37.292	1.00	249.69
	5662 5663	CD	GLU D	132	24.762	50.658	36.806	1.00	249.69
	5664	OE1	GLU D	132	25.408	51.508	37.461	1.00	249.69
70	5665	OE2	GLU D	132	24.106	50.945	35.777	1.00	249.69
• •									

		•	OLU D	132	27.976	47.929	39.090	1.00	246.45
	5666	C	GLU D	132	27.639	47.527	40.210	1.00	246.45
	5667	0	ASN D	133	29.219	48.320	38.821	1.00	125.13
	5668	N CA	ASN D	133	30.220	48.146	39.877	1.00	125.13
5	5669	CA ·	ASN D	133	31.670	48.261	39.299	1.00	124.76
2	5670	CB CG	ASN D	133	32.189	49.671	39.168	1.00	124.76
	5671	OD1	ASN D	133	31.488	50.569	38.725	1.00	124.76
	5672	ND2	ASN D	133	33.462	49.855	39.512	1.00	124.76
	5673		ASN D	133	30.069	48.859	41.223	1.00	125.13
10	5674	C	ASN D	133	29.046	49.479	41.527	1.00	125.13
10	5675	N	HIS D	134	31.077	48.688	42.057	1.00	175.64
	5676	CA	HIS D	134	31.054	49.259	43.375	1.00	175.64
	5677 5678	CB	HIS D	134	30.511	48.218	44.358	1.00	249.69
	5679	CG	HIS D	134	30.264	48.759	45.738	1.00	249.69
15	5680	CD2	HIS D	134	30.834	48.440	46.925	1.00	249.69
13	5681	ND1	HIS D	134	29.361	49.759	45.988	1.00	249.69
	5682	CE1	HIS D	134	29.377	50.048	47.287	1.00	249.69
	5683	NE2	HIS D	134	30.260	49.263	47.870	1.00	249.69
	5684	Ċ	HIS D	134	32.481	49.650	43.733	1.00	175.64
20	5685	ŏ	HIS D	134	33.352	49.738	42.862	1.00	175.64
20	5686	Ň	ASN D	135	32.714	49.878	45.020	1.00	171.27
	5687	CA	ASN D	135	34.020	50.269	45.510	1.00	171.27
	5688	CB	ASN D	135	34.116	51.799	45.567	1.00	249.69
	5689	ÇĞ	ASN D	135	34.113	52.439	44.180	1.00	249.69
25	5690	OD1	ASN D	135	34.830	51.972	43.295	1.00	249.69
23	5691	ND2	ASN D	135	33.336	53.512	43.992	1.00	249.69
	5692	C	ASN D	135	34.237	49.660	46.894	1.00	171.27
	5693	ō	ASN D	135	34.009	50.303	47.907	1.00	171.27
	5694	N	ILE D	136	34.670	48.405	46.916	1.00	141.21
30	5695	CA	ILE D	136	34.953	47.636	48.143	1.00	141,21
•	5696	CB	ILE D	136	35.894	46.432	47.813	1.00	122.14
	5697	CG2	ILE D	136	37.169	46.918	47.141	1.00	122.14
	5698	CG1	ILE D	136	36.246	45.665	49.068	1.00	122.14
	5699	CD1	ILE D	136	37.202	44.530	48.789	1.00	122.14
35	5700	С	ILE D	136	35.571	48.458	49.276	1.00	141.21 141.21
	5701	0	ile d	136	36.769	48.809	49.257	1.00	155.34
	5702	N	SER D	137	34.751	48.728	50.282	1.00 1.00	155.34
	5703	CA	SER D	137	35.189	49.539	51.415 51.662	1.00	178.90
	5704	CB	SER D	137	34.179	50.648	51.884	1.00	178.90
40	5705	OG.	SER D	137	34.452	51.311	52.739	1.00	155.34
	5706	Ç	SER D	137	35.447	48.817 47.815	53.067	1.00	155.34
	5707	0	SER D	137	34.804 36.378	49.372	53.509	1.00	165.15
	5708	N	ILE D	138 138	36.770	48.823	54.792	1.00	165.15
45	5709	CA	ILE D	138	38.095	48.075	54.654	1.00	128.87
45	5710	CB CG2	ILE D	138	38.690	47.804	56.022	1.00	128.87
	5711	ÇG1	ILE D	138	37.861	46.780	53.894	1.00	128.87
	5712 5713	CD1	ILE D	138	39.131	46.098	53.483	1.00	128.87
	5713 5714	C.	ILE D	138	36.919	49.901	55.863	1.00	165.15
50	571 4 5715	ŏ	ILE D	138	37.703	50.849	55.720	1.00	165.15
50	5716	Ň	THR D	139	36.167	49.733	56.944	1.00	191.18
	5717	CA.	THR D	139	36.186	50.663	58.065	1.00	191.18
	5718	CB	THR D	139	34.891	50.533	58.855	1.00	246.32
	5719	OG1	THR D	139	34.694	49.160	59.210	1.00	246.32
55	5720	CG2	THR D	139	33.713	50.988	58.006	1.00	246.32
33	5721	Č	THR D	139	37.364	50.342	58.976	1.00	191.18
	5722	ŏ	THR D	139	38.413	50.981	58.911	1.00	191.18
	5723	Ň	ASN D	140	37.173	49.343	59.827	1.00	193.50
	5724	CA	ASN D	140	38.211	48.887	60.742	1.00	193.50
60	5725	CB	ASN D	140	37.561	48.246	61.967	1.00	183.46
•	5726	CG	ASN D	140	38.567	47.701	62.943	1.00	183.46
	5727	OD1	ASN D	140	39.474	46.972	62.554	1.00	183.46
	5728	ND2	ASN D	140	38.403	48.038	64.218	1.00	183.46
	5729	C	ASN D	140		47.849	59.960	1.00	193.50
65	5730	0	ASN D	140		46.846	59.482	1.00	193.50
	5731	N	ALA D	141	40.324	48.088	59.822	1.00	163.85
	5732	CA	ALA D	141	41.190	47.179	59.061	1.00	163.85
	5733	CB	ALA D	141		48.002	58.187	1.00	57.61
	5734	Ç	ALA D	141		46.131	59.872	1.00	163.85
70	5735	0	ALA D	141	42.669	46.446	60.823	1.00	163.85

				•					
	5736	N	THR D	142	41.794	44.880	59.470	1.00	158.30
		ČA	THR D	142	42.464	43.765	60.113	1.00	158.30
	5737			142	41.654	42.471	59.957	1.00	191.01
	5738	CB:	THR D			42.703	60.352	1.00	191.01
_	5739	OG1	THR D	142	40.299	41.370	60.813	1.00	
5	5740	CG2	THR D	142	42.248				191.01
-	5741	С	THR D	142	43.798	43.568	59.407	1.00	158.30
	5742	0	THR D	142	43.992	44.042	58.282	1.00	158.30
	5743	Ň	VAL D	143	44.723	42.867	60.052	1.00	168.28
		CA	VAL D	143	46.017	42.637	59. 43 0	1.00	168.28
10	5744		VAL D	143	47.063	42.169	60.441	1.00	249.69
10	5745	CB	VAL D	143	46.777	40.734	60.851	1.00	249.69
	5746	CG1			48.453	42.298	59.830	1.00	249.69
	5747	CG2	VAL D	143		41.580	58. 35 7	1.00	168.28
	5748	С	VAL D	143	45.893				
	5749	0	VAL D	143	46.711	41.521	57.446	1.00	168.28
15	5750	N	GLU D	144	44.874	40.737	58.469	1.00	197.52
	5751	CA	GLU D	144	44.671	39.694	57.475	1.00	197.52
	5752	СВ	GLU D	144	43.667	38.654	57. 96 5	1.00	249.69
		CG	GLU D	144	44.088	37.957	59.232	1.00	249.69
	5753		GLU D	144	43.210	38.332	60.397	1.00	249.69
	5754	CD		144	41.994	38.051	60.329	1.00	249.69
20	5755	OE1	GLU D			38.910	61.376	1.00	249.69
	5756	OE2	GLU D	144	43.729		56.1 54	1.00	197.52
	5757	С	GLU D	144	44.186	40.286			
	5758	0	GLU D	144	44.159	39.591	55.137	1.00	197.52
	5759	N	ASP D	145	43.805	41.565	56.173	1.00	135.76
25	5760	CA	ASP D	145	43.346	42.243	54.965	1.00	135.76
23	5761	CB	ASP D	145	42.617	43.538	55.311	1.00	217.88
		CG	ASP D	145	41.206	43.293	55.813	1.00	217.88
	5762			145	40.415	42.658	55.081	1.00	217.88
	5763	OD1	ASP D		40.881	43.737	56.938	1.00	217.88
	5764	OD2	ASP D	145		42.549	54.030	1.00	135.76
30	5765	С	ASP D	145	44.512			1.00	135.76
	5766	0	ASP D	145	44.319	42.840	52.851		
	5767	N	SER D	146	45.728	42.478	54.559	1.00	129.49
	5768	CA	SER D	146	46. 9 45	42.736	53.778	1.00	129.49
	5769	СВ	SER D	146	48.185	42.741	54.696	1.00	138.30
35	5770	OG	SER D	146	48.092	43.709	55.730	1.00	138.30
55	5771	Č	SER D	146	47.128	41.662	52.70 9	1.00	129.49
	5772	ŏ	SER D	146	47.094	40.471	53.005	1.00	129.49
	5773	Ň	GLY D	147	47.335	42.079	51.466	1.00	156.91
		CA	GLY D	147	47.534	41.109	50.400	1.00	156.91
40	5774		GLY D	147	47.729	41.750	49.041	1.00	156.91
40	5775	C		147	48.071	42.922	48.948	1.00	156.91
	5776	0	GLY D		47.514	40.983	47.980	1.00	120.73
	5777	N	THR D	148		41.506	46.626	1.00	120.73
	5778	CA	THR D	148	47.663			1.00	132.18
	5779	CB	THR D	148	48.770	40.742	45.861		
45	5780	OG1	THR D	148	48.194	39.716	45.043	1.00	132.18
	5781	CG2	THR D	148	49.728	40.096	46.837	1.00	132.18
	5782	C	THR D	148	46.320	41.438	45. 84 8	1.00	120.73
	5783	ŏ	THR D	148	45.808	40.338	45.526	1.00	120.73
		Ň	TYR D	149	45.757	42.618	45. 5 45	1.00	89.32
50	5784		TYR D	149	44.471	42.706	44.849	1.00	89.32
50	5785	CA		149	43.573	43.748	45.540	1.00	105.54
	5786	CB	TYR D		43.303	43.551	47.020	1.00	105.54
	5787	CG	TYR D	149	44.004		47.984	1.00	105.54
	5788	CD1	TYR D	149	44.281	43.842			105.54
	5789	CE1	TYR D	149	44.016	43.690	49.350	1.00	
55	5790	CD2	TYR D	149	42.056	43.098	47.460	1.00	105.54
	5791	CE2	TYR D	149	41.781	42.942	48.812	1.00	105.54
	5792	CZ	TYR D	149	42.761	43.237	49.747	1.00	105.54
	5793	ŎĤ	TYR D	149	42.470	43.085	51.077	1.00	105.54
		Ċ,	TYR D	149	44.565	43.068	43.360	1.00	89.32
۲0	5794		TYR D	149	45.586	43.579	42.877	1.00	89.32
60		0			43.462	42.806	42.662	1.00	127.86
	5796	N.	TYR D	150			41.246	1.00	127.86
	5797	ÇA	TYR D	150	43.278	43.117	40.355	1.00	148.19
	5798	CB	TYR D	150	44.146	42.218			148.19
	5799	CG	TYR D	150	43.643	40.801	40.109	1.00	
65	5800	CD1	TYR D	150	42.539	40.554	39.296	1.00	148.19
-	5801	CE1	TYR D	150	42.105	39.243	39.025	1.00	148.19
	5802	CD2	TYR D	150		39.701	40.649	1.00	148.19
	5803	CE2	TYR D	150		38.381	40.378	1.00	148.19
		CZ	TYR D	150		38.163	39.563	1.00	148.19
70	5804	OH	TYR D	.150		36.876	39.273	1.00	148.19
70	5805	Un	LIN D	.100					

	5000	<u> </u>	TYR D	150	41.790	42.882	40.976	1.00	127.86
	5806 5807	C	TYR D	150	41.157	42.091	41.681	1.00	127.86
	5808	N ·	CYS D	151	41.218	43.567	39.987	1.00	122.94
	5809	CA	CYS D	151	39.793	43.385	39.685	1.00	122.94
5	5610	Č	CYS D	151	39.559	43.047	38.224	1.00	122.94
-	5811	ŏ	CYS D	151	40.438	43.275	37.379	1.00	122.94
	5812	СB	CYS D	151	39.010	44.640	40.049	1.00	183.39
	5813	SG	CYS D	151	39.522	46.144	39.169	1.00	183.39
	5814	N	THR D	152	38.379	42.494	37.935	1.00	139.21
10	5815	CA	THR D	152	38.013	42.119	36.565	1.00	139.21
-	5816	СВ	THR D	152	37.955	40.598	36.383	1.00	172.57
	5817	OG1	THR D	152	36.776	40.090	37.025	1.00	172.57
	5818	CG2	THR D	152	39.185	39.945	36.985	1.00	172.57
	5819	Ç	THR D	152	36.627	42.660	36.247	1.00	139.21
15	5820	0	THR D	152	35.765	42.721	37.124	1.00 1.00	139.21 182.81
	5821	N _.	GLY D	153	36.411	43.037 43.562	34.993 34.620	1.00	182.81
	5822	CA	GLY D	153	35.115	43.665	33.126	1.00	182.81
	5823	C	GLY D	153	34.905	43.520	32.350	1.00	182.81
20	5824	0	GLY D LYS D	153 154	35.844 33.662	43.917	32.730	1.00	140.36
20	5825	N	LYS D Lys d	154	33.307	44.047	31.327	1.00	140.36
	5826	CA CB	LYS D	154	32.064	43.211	31.040	1.00	249.69
	5827 5828	CG	LYS D	154	31.649	43.177	29.581	1.00	249.69
	5829	CD	LYS D	154	30.442	42.266	29.384	1.00	249.69
25	5830	CE	LYS D	154	29.973	42.264	27.938	1.00	249.69
23	5831	NZ	LYS D	154	28.786	41.385	27.740	1.00	249.69
	5832	Ċ	LYS D	154	33.055	45.519	30.936	1.00	140.36
	5833	ŏ	LYS D	154	32,150	46.184	31.458	1.00	140.36
	5834	Ň	VAL D	155	33.881	46.020	30.021	1.00	200.49
30	5835	CA	VAL D	155	33.793	47.390	29.517	1.00	200.49
	5836	СВ	VAL D	155	35.198	48.038	29.434	1.00	172.58
	5837	CG1	VAL D	155	35.116	49.415	28.834	1.00	172.58
	5838	CG2	VAL D	155	35.811	48.111	30.820	1.00	172.58
	5839	С	VAL D	155	33.211	47.276	28.116	1.00	200.49
35	5840	0	VAL D	155	33.711	46.504	27.298	1.00 1.00	200.49 193.00
	5841	N	TRP D	156	32.169	48.051	27.831 26.522	1.00	193.00
	5842	CA	TRP D	156	31.502	47.986 48.222	25.344	1.00	249.69
	5843	CB	TRP D	156 156	32.472 33.061	49.610	25.206	1.00	249.69
40	5844	CG CD2	TRP D	156	32.372	50.817	24.849	1.00	249.69
40	5845 5846	CE2	TRP D	156	33.330	51.857	24.815	1.00	249.69
	5847	CE3	TRP D	156	31.047	51.121	24.550	1.00	249.69
	5848	CD1	TRP D	156	34.372	49.961	25.377	1.00	249.69
	5849	NE1	TRP D	156	34.537	51.309	25.141	1.00	249.69
45	5850	CZ2	TRP D	156	32.996	53.172	24.499	1.00	249.69
	5851	CZ3	TRP D	156	30.729	52.433	24.235	1.00	249.69
	5852	CH2	TRP D	156	31.692	53.438	24.219	1.00	249.69
	5853	С	TRP D	156	30.980	46.564	26.418	1.00	193.00
	5854	0	TRP D	156	29.921	46.232	26.957	1.00	193.00
50	5855	N	GLN D	157	31.755	45.727	25.732	1.00	206.01
	5856	CA	GLN D	157	31.402	44.330	25.555	1.00	206.01
	5857	CB	GLN D	157	30.644	44.150	24.236	1.00	249.69
	5858	CG	GLN D	157	29.201	44.650	24.285	1.00 1.00	249.69 249.69
	5859	CD	GLN D	157	28.329	43.857 42.651	25.262 25.090	1.00	249.69
55	5860	OE1	GLN D	157	28.115	44.535	26.291	1.00	249.69
	5861	NE2	GLN D	157	27.820 32.585	43.353	25.631	1.00	206.01
	5862	C	GLN D	157	32.508	42.233	25.122	1.00	206.01
	5863	0 N	GLN D LEU D	157 158	33.674	43.773	26.269	1.00	203.26
60	5864 5865	CA	LEU D	158	34.833	42.900	26.427	1.00	203.26
QQ.	5866	CB	LEU D	158	35.991	43.350	25.529	1.00	242.89
	5867	ČĠ	LEU D	158	35.914	43.035	24.033	1.00	242.89
	5868	CD1	LEU D	158	37.324	42.735	23.537	1.00	242.89
	58 6 9	CD2	LEU D	158	35.015	41.829	23.772	1.00	242.89
65	5870	C	LEU D	158	35.301	42.846	27.878	1.00	203.26
35	5871	ŏ	LEU D	158	35.127	43.802	28.629	1.00	203.26
	5872	Ň	ASP D	159	35.886	41.718	28.268	1.00	176.99
	5873	CA	ASP D	159	36.376	41.545	29.629	1.00	176.99
	5874	CB	ASP D	159	36.361	40.068	30.005	1.00	232.53
70	5875	CG	ASP D	159	35.012	39.424	29.781	1.00	232.53

	5876	OD1	ASP D	159	34.036	39.849	30.434	1.00	232.53
	5877	OD2	ASP D	159	34.929	38.495	28.950	1.00	232.53
	5878	С	ASP D	159	37.805	42.075	29.760	1.00	176.9 9
	5879	0	ASP D	159	38.590	42.025	28.810	1.00	176.99
5	5880	N	TYR D	160	38.143	42.588	30.938	1.00	175.60
_	5881	CA	TYR D	160	39.484	43.102	31.170	1.00	175.60
	5882	СВ	TYR D	160	39.559	44.592	30.873	1.00	205.83
	5883	CG	TYR D	160	39.112	44.956	29.483	1.00	205.83
	5884	CD1	TYR D	160	37.778	45.271	29.216	1.00	205.83
10	5885	CE1	TYR D	160	37.361	45. 63 6	27.939	1.00	205.83
••	5886	CD2	TYR D	160	40.022	45.009	28.435	1.00	205.83
	5887	CE2	TYR D	160	39.614	45.373	27.148	1.00	205.83
	5888	CZ	TYR D	160	38.284	45.687	26.912	1.00	205.83
	5889	OH	TYR D	160	37.883	46.070	25.658	1.00	205.83
15	5890	Č.	TYR D	160	39.941	42.855	32.593	1.00	175.60
13	5891	ŏ	TYR D	160	39.151	42.853	33.545	1.00	175.60
	5892	Ň	GLU D	161	41.243	42.653	32.718	1.00	144.68
	5893	ĊA	GLU D	161	41.879	42.385	33.998	1.00	144.68
	5894	CB	GLU D	161	42.697	41.094	33.859	1.00	232.05
20	5895	ČĞ	GLU D	161	43.497	40.642	35.071	1.00	232.05
20	5896	CD	GLU D	161	43.969	39.194	34.942	1.00	232.05
	5897	OE1	GLU D	161	44.936	38.819	35.643	1.00	232.05
	5898	OE2	GLU D	161	43.363	38.430	34.151	1.00	232.05
		C	GLU D	161	42,759	43.587	34.344	1.00	144.68
25	5899		GLU D	161	43.353	44.206	33.459	1.00	144.68
23	5900	0	SER D	162	42.814	43.922	35.628	1.00	134.82
	5901	N		162	43.594	45.064	36.101	1.00	134.82
	5902	CA	SER D			45.712	37.288	1.00	129.75
	5903	CB	SER D	162	42.881	44.801	38.381	1.00	129.75
20	5904	OG	SER D	162	42.767 44.983	44.669	36.541	1.00	134.82
30	5905	C	SER D	162	45.221	43.504	36.838	1.00	134.82
	5906	Ö	SER D	162		45.634	36.581	1.00	145.43
	5907	N	GLU D	163	45.898	45.334 45.334	37.050	1.00	145.43
	5908	CA	GLU D	163	47.238	46.575	36. 96 4	1.00	249.69
ás	5909	CB	GLU D	163	48.133	46.949	35.552	1.00	249.69
35	5910	CG	GLU D	163	48.587	46.008	35.001	1.00	249.69
	5911	CD	GLU D	163	49.651	45.850	35.650	1.00	249.69
	5912	OE1	GLU D	163	50.709		33.917	1.00	249.69
	5913	OE2	GLU D	163	49.433	45.429	38.519	1.00	145.43
40	5914	C	GLU D	163	47.047	44.921 45.384	39.168	1.00	145.43
40	5915	0	GLU D	163	46.101			1.00	113.31
	5916	N	PRO D	164	47.906	44.037	39.057		144.09
	5917	CD	PRO D	164	48.999	43.317	38.369	1.00 1.00	113.31
	5918	CA	PRO D	164	47.794	43.578	40.447		
4.5	5919	CB	PRO D	164	48.555	42.277	40.434	1.00	144.09
45	5920	ÇG	PRO D	164	49.685	42.607	39.519	1.00	144.09
	5921	C	PRO D	164	48.395	44.576	41.422	1.00	113.31
	5922	Ö	PRO D	164	49.399	45.229	41.095	1.00	113.31
	5923	N	LEU D	165	47.807	44.679	42.613	1.00	104.79
~~	5924	CA	LEU D	165	48.305	45.642	43.591	1.00	104.79
50	5925	CB	LEU D	165	47.329	46.816	43.687	1.00	127.61
	5926	CG	LEU D	165	47.719	47.920	44.665	1.00	127.61
	5927	CD1	LEU D	165	49.250	48.130	44.649	1.00	127.61
	5928	CD2	LEU D	165	46.959	49.193	44.283	1.00	127.61
	5929	Ç	LEU D	165	48.560	45.097	44.980	1.00	104.79
55	5930	0	LEU D	165	47.691	44.427	45.545	1.00	104.79
	5931	N	ASN D	166	49.739	45.405	45.533	1.00	129.66
	5932	CA	ASN D	166	50.090	44.944	46.878	1.00	129.66
	5933	CB	ASN D	166	51.594	44.769	47.024	1.00	189.08
	5934	CG	ASN D	166	52. 05 0	43.354	46.741	1.00	189.08
60	5935	OD1	ASN D	166	51 <i>.2</i> 75	42.407	46.867	1.00	189.08
	5936	ND2	asn d	166	53.324	43.209	46.381	1.00	189.08
	5937	C	ASN D	166	49.612	45.924	47.955	1.00	129.66
	5938	0	ASN D	166	49.610	47.138	47.755	1.00	129.66
	5939	N	ILE D	167	49.221	45.387	49.105	1.00	126.98
65	5940	CA	ILE D	167	48.731	46.196	50.211	1.00	126.98
	5941	СВ	ILE D	167	47.211	48.242	50.220	1.00	113.09
	5942	CG2	ILE D	167	46.740	46.998	51.438	1.00	113.09
	5943	CG1	ILE D	167	46.716	46.889	45.940	1.00	113.09
	5944	CD1	ILE D	167	45.225	46.900	48.843	1.00	113.09
70	5945	С	ILE D	167	49.185	45.645	51.555	1.00	126.98

						•			
	5040	^	ILE D	167	48.978	44.480	51.875	1.00	126.98
	5946	O N	THR D	168	49.769	46.499	52.369	1.00	123.13
	5947 5948	CA CA	THR D	168	50.238	46.029	53.647	1.00	123.13
	5 94 9	CB	THR D	168	51.761	46.052	53.678	1.00	145.39
5	5950	OG1	THR D	168	52.253	45.258	52.593	1.00	145.39
J	5951	CG2	THR D	168	52.281	45.490	54.987	1.00	145.39
	5952	C	THR D	168	49.695	46.76 6	54.864	1.00	123.13
	5953	0	THR D	168	49.839	47.983	55.000	1.00	123.13
	5954	N	VAL D	169	49.061	46.004	55.748	1.00	129.26
10	5955	CA	VAL D	169	48.501	46.536	56.981	1.00	129.26
	5956	CB	VAL D	169	47.067	45.982	57.209	1.00	119.28
	5 95 7	CG1	VAL D	169	46.683	46.096	58.653	1.00	119.28
	5958	CG2	VAL D	169	46.065	46.769	56.377	1.00 1.00	119.28 129.26
	5959	Ç	VAL D	169	49.439	46.104	58.098 58.419	1.00	129.26
15	5960	0	VAL D	169	49.525	44.914 47.069	58.664	1.00	108.63
	5961	N	ILE D	170	50.162 51.111	46.798	59.750	1.00	108.63
	5962	CA	ILE D	170 170	52.340	47.687	59.607	1.00	169.72
	5963	CB	ILE D	170	52.891	47.560	58.200	1.00	169.72
20	5964	CG2 CG1	ILE D	170	51.963	49.148	59.833	1.00	169.72
20	5965 5066	CD1	ILE D	170	53.138	50.116	59.741	1.00	169.72
	5966 5967	C	ILE D	170	50.448	47.058	61.111	1.00	108.63
	5968	ŏ	ILE D	170	49.389	47.687	61.170	1.00	108.63
	5969	Ň	LYS D	171	51.044	46.600	62.206	1.00	180.64
25	5 97 0	ČA	LYS D	171	50.427	46.811	63.518	1.00	180.64
23	5971	CB	LYS D	171	50.095	45.460	64.130	1.00	216.97
	5972	CG	LYS D	171	51.300	44.550	64.204	1.00	216.97
	5973	CD	LYS D	171	50.911	43.084	64.180	1.00	216.97
	5974	CE	LYS D	171	49.997	42.721	65.338	1.00	216.97
30	5975	NZ	LYS D	171	49.677	41.265	65.351	1.00	216.97
	5976	С	LYS D	171	51 <i>.2</i> 77	47.623	64.496	1.00	180.64
	5977	0	LYS D	171	50.952	47.715	65.686	1.00	180.64
	5978	C1	NAG D	221	40.588	68.345	34.460 34.228	1.00 1.00	249.69 249.69
	5979	C2	NAG D	221	39.263	67.620	34.156	1.00	249.69
35	5980	N2	NAG D	221	39.503	66.190 65.328	34.426	1.00	249.69
	5981	C7	NAG D	221 221	38.524 37.379	65.680	34.734	1.00	249.69
	5982	O7	nag d Nag d	221	38.865	63.847	34.336	1.00	249.69
	5983	C8 C3	NAG D	221	38.607	68.107	32,935	1.00	249.69
40	5984 5985	G3	NAG D	221	37.303	67.542	32.815	1.00	249.69
40	5986	24	NAG D	221	38.508	69.645	32.882	1.00	249.69
	5987	04	NAG D	221	38.122	70.004	31.534	1.00	249.69
	5988	C5	NAG D	221	39.874	70.288	33.238	1.00	249.69
	5989	O 5	NAG D	221	40.374	69.764	34.489	1.00	2 (9.69
45	5990	C6	NAG D	221	39.806	71. 79 7	33.398	1.00	249.69
	5991	06	NAG D	221	38.830	72.175	34.359	1.00	249.69
	5992	C1	NAG D	222	37.598	71.265	31.271	1.00	249.69
	5993	C2	NAG D	222	36.393	71.128	30.316	1.00	249.69
	5994	N2	NAG D	222	35.353	70.322	30.940	1.00	249.69
50	5995	C7	NAG D	222	34.138	70.826	31.159	1.00	249.69
	5996	07	NAG D	222	33.821	71.980	30.854	1.00 1.00	249.69 249.69
	5997	C8	NAG D	222	33.115	69.911 70.476	31.816		- 40 00
	5998	cs	NAG D	222	36.853	70.476 70.461	28.991 28.055	. 1.00 1.00	249.69 249.69
	5999	03	NAG D	222	35.784	70.461 71.236	28.392	1.00	249.69
55	6000	C4	nag d Nag d	222 222	38.047 38.552	70.527	27.265	1.00	249.69
	6001	04 05	NAG D	222	39.161	71.402	29.445	1.00	249.69
	6002	C5 O5	NAG D	222	38.632	72.044	30.639	1.00	249.69
	6003 6004	C 8	NAG D	222	40.342	72.235	28.961	1.00	249.69
60	6005	06	NAG D	222	41.578	71.582	29.216	1.00	249.69
w	6006	C1	NAG D	242	60.393	61.563	38.161	1.00	217.32
	6007	C2	NAG D	242	60.080	62.065	36.753	1.00	217.32
	6008	N2	NAG D	242	59.542	63.410	36.776	1.00	217.32
	6009	C7	NAG D	242	60.185	64.390	36.140	1.00	217.32
65	6010	0 <i>7</i>	NAG D	242	61.243	64.215	35.527	1.00	217.32
55	6011	Č8	NAG D	242	59.572	65.781	36.193	1.00	217.32
	6012	C3	NAG D	242	59.090	61.109	36.102	1.00	217.32
	6013	03	NAG D	242	58.789	61.543	34.778	1.00	217.32
	6014	C4	NAG D	242		59. 697	36.072	1.00	217.32
70	6015	04	NAG D	242	58.682	58:764	35.604	1.00	217.32

			****	046	CO 470	59.270	37.475	1.00	217.32
	6016	C5	NAG D	242 242	60.173 61.023	60.283	38.071	1.00	217.32
	6017	O5 C6	nag d Nag d	242	61.023	57.999	37.419	1.00	217.32
	6018	C6 O6	NAG D	242	60.329	56.906	38.029	1.00	217.32
5	6019 6020	C1	NAG D	243	58.975	58.047	34.449	1.00	249.32
J	6021	C2	NAG D	243	58.093	56.797	34.373	1.00	249.32
	6022	N2	NAG D	243	58.304	55.934	35.517	1.00	249.32
	6023	C7	NAG D	243	57.260	55.458	36.184	1.00	249.32
	6024	07	NAG D	243	56.095	55.727	35.887	1.00	249.32
10	6025	C8	NAG D	243	57.553	54,550	37.368	1.00	249.32
	6026	C3	NAG D	243	58.410	56.048	33.091	1.00	249.32 249.32
	6027	03	NAG D	243	57.609	54.878 56.960	32.999 31.920	1.00 1.00	249.32 249.32
	6028	C4	NAG D	243 243	58.125 58.387	56.198	30.758	1.00	249.32
15	6029	04 05	NAG D NAG D	243	58.994	58.245	32.040	1.00	249.32
13	6030 6031	C5 O5	NAG D	243	58.710	58.893	33.315	1.00	249.32
	6032	C6	NAG D	243	58.695	59.274	30.969	1.00	249.32
	6033	0 6	NAG D	243	57.361	59.747	31.063	1.00	249.32
	6034	C1	MAN D	244	57.701	56.400	29.5 9 1	1.00	249.69
20	6035	C2	MAN D	244	58. 76 4	56.236	28.599	1.00	249.69
	6036	O2	MAN D	244	59.572	55.101	28.964	1.00	249.69
	6037	C3	MAN D	244	58.183	56.214	27.213	1.00	249.69 249.69
	6038	·O3	MAN D	244	59.205	56.198 55.086	26.236 27.057	1.00 1.00	249.69 249.69
25	6039	C4	MAN D	244 244	57.187 56.690	55.063	25.730	1.00	249.69
25	6040	O4 C5	MAN D MAN D	244	56.059	55.334	28.066	1.00	249.69
	6041 6042	O5	MAN D	244	56.637	55.331	29.433	1.00	249.69
	6043	C6	MAN D	244	54.855	54.371	27.914	1.00	249.69
	6044	06	MAN D	244	55.056	53.129	28.567	1.00	249.69
30	6045	C1	NAG D	250	45.970	78.192	45.348	1.00	249.69
	6046	C2	NAG D	250	44.549	78.482	45.867	1.00	249.69
	6047	N2	NAG D	250	44.538	78.485	47.317 47.981	1.00 1.00	249.69 249.69
	6048	C7	NAG D	250	44.384 44.241	79.627 80.713	47.415	1.00	249.69
35	6049	O7 C8	NAG D NAG D	250 250	44.386	79.553	49.506	1.00	249.69
33	6050 6051	C3	NAG D	250	43.581	77.413	45.337	1.00	249.69
	6052	os os	NAG D	250	42.249	77.716	45.732	1.00	249.69
	6053	C4	NAG D	250	43.666	77.341	43.807	1.00	249.69
	6054	O4	NAG D	250	42,863	76.265	43.339	1.00	249.69
40	6055	C 5	NAG D	250	45.136	77.138	43.368 43.916	1.00 1.00	249.69 249.69
	6056	O5	NAG D	250	45.975 45.334	78.187 77.155	43.916	1.00	249.69
	6057	C6 O6	nag d Nag d	250 250	46.706	77.133	41.513	1.00	249.69
	6058 6059	C1	NAG D	274	64.018	69.436	61.817	1.00	249.69
45	6060	C2	NAG D	274	63.805	68.308	62.845	1.00	249.69
10	6061	N2	NAG D	274	62.614	68.567	63.639	1.00	249.69
	6062	C7	NAG D	274	61.945	67.559	64.201	1.00	249.69
	6063	07	NAG D	274	62.289	66.377	64.093	1.00	249.69 249.69
50	6064	C8	NAG D	274	60.707	67.911 69.104	65.011 63.760	1.00 1.00	249.69
50	6065	C3	NAG D	274 274	65.040 64.908	68.194 67.066	64.619	1.00	249.69
	6066	O3 C4	NAG D NAG D	274	66.321	68.053	62.922	1.00	249.69
	6067 6068	64	NAG D	274	67.463	68.083	63.776	1.00	249.69
	6068 6069	C5	NAG D	274	66.405	69.191	61.890	1.00	249.69
55	6070	O5	NAG D	274	65.217	69.199	61.060	1.00	249.69
••	6071	C6	NAG D	274	67.605	69.054	60.964	1.00	249.69
	6072	Q6	NAG D	274	67.558	70.006	59.911	1.00	249.69
	6073	C1	NAG D	335	33.933	54.753	43.517 44.462	1.00 1.00	249.69 249.69
60	6074	C2	NAG D	335 335	33.681 33.369	55.966 55.476	45.797	1.00	249.69
60	6075	N2 C7	NAG D NAG D	335	34.175	55.736	46.826	1.00	249.69
	6076 6077	07 07	NAG D	335	35.208	56.398	46.727	1.00	249.69
	6078	C8	NAG D	335	33.768	55.178	48.177	1.00	249.69
	6079	čš	NAG D	335	32.547	56.909	44.003	1.00	249.69
65	6080	O 3	NAG D	335	32.693	58.170	44.644	1.00	249.69
	6081	C4	NAG D	335	32.568	57.114	42.494	1.00	249.69
	6082	04	NAG D	335	31.469	57.925 55.747	42.098	1.00	249.69 249.69
	6083	C5	NAG D	335 335	32.490 33,699	55.747 55.014	41.830 42.109	1.00 1.00	249.69 249.69
70	6084 6085	O5 C6	NAG D NAG D	335 335	32.365	55.844	40.319	1.00	249.69
70	0 000	•	itag D						

	6086	O6	NAG D	335	31.232	55.131	20 050	4.00	
	6087	C1	NAG D	340	38.129	47.005	39.850 65.199	1.00 1.00	249.69
	6088	C2	NAG D	340	39.319	46.805	66.150	1.00	249.69
_	6089	N2	NAG D	340	40.524	46.521	65.388	1.00	249.69 249.69
5	6090	C7	NAG D	340	41.665	47.160	65.655	1.00	249.69
	6091	O7	NAG D	340	41.779	48.007	66.549	1.00	249.69
	6092 6093	C8 C3	NAG D	340	42.871	46.799	64.801	1.00	249.69
	6094	03	NAG D NAG D	340 340	39.000 40.042	45.640 45.490	67.106	1.00	249.69
10	6095	C4	NAG D	340	37.670	45.482 45.894	68.064 67.828	1.00	249.69
	6096	04	NAG D	340	37.324	44.743	68.593	1.00 1.00	249.69
	6097	C5	NAG D	340	36.556	46.207	66.801	1.00	249.69 249.69
	6098	O 5	NAG D	340	36.949	47.307	65.948	1.00	249.69
15	6099	C6	NAG D	340	35.226	46.591	67.427	1.00	249.69
15	6100 6101	O6 C1	NAG D NAG D	340	34.319	47.067	66.440	1.00	249.69
	6102	C2	NAG D	366 366	53.829 54.811	41.917	45.964	1.00	214.56
	6103	N2	NAG D	366	54.141	42.093 42.757	44.812 43.705	1.00	214.56
	6104	C 7	NAG D	366	54.172	44.086	43.595	1.00 1.00	214.56 214.56
20	6105	O 7	NAG D	366	54.769	44.819	44.386	1.00	214.56
	6106	C8	NAG D	366	53.436	44.705	42.413	1.00	214.56
	6107	C3	NAG D	366	55.328	40.725	44.367	1.00	214.56
	6108 6109	O3 C4	NAG D NAG D	366	56.374	40.896	43.416	1.00	214.56
25	6110	04	NAG D	366 366	55.847 56.067	39.896	45.553	1.00	214.56
	6111	C5	NAG D	366	54.830	38.537 39.900	45.104 46.709	1.00 1.00	214.56
	6112	O5	NAG D	366	54.471	41.245	47.050	1.00	214.56
	6113	C6	NAG D	366	55.334	39.248	47.980	1.00	214.56 214.56
20	6114	O 6	NAG D	366	54.292	39.118	48.934	1.00	214.56
30	6115	C1	NAG D	367	57.323	37.987	45.329	1.00	231.83
	6116 6117	C2 N2	nag d Nag d	367	57.238	36.462	45.283	1.00	231.83
	6118	C7	NAG D	367 367	56.271 55.141	35.974 35.410	46.246	1.00	231.83
	6119	07	NAG D	367	54.861	35.279	45.821 44.620	1.00 1.00	231.83
35	6120	C8	NAG D	367	54.169	34.918	46.887	1.00	231.83 231.83
	6121	C3	NAG D	367	58.627	35.898	45.572	1.00	231.83
	6122	03	NAG D	367	58.601	34.478	45.528	1.00	231.83
	6123 6124	C4 O4	NAG D	367	59.611	36.433	44.526	1.00	231.83
40	6125	C5	nag d Nag d	367 367	60.922 59.572	35.989	44.845	1.00	231.83
	6126	O5	NAG D	367	58.216	37.974 38.443	44.486 44.296	1.00 1.00	231.83
	6127	C6	NAG D	367	60.403	38.550	43.358	1.00	231.83 231.83
	6128	O6	NAG D	367	59.584	39.177	42.385	1.00	231.83
45	6129	CB	LYS E	4	8.883	64.586	0.000	1.00	249.69
43	6130 6131	CD	LYS E	4	7.510	64.141	-0.503	1.00	249.69
	6132	CE	LYS E Lys e	4 4	6.532	63.873	0.645	1.00	249.69
	6133	NZ	LYS E	••	5.149 4.173	63.459 63.179	0.123 1.220	1.00	249.69
	6134	Ċ	LYS E	4	9.271	66.045	-1.989	1.00 1.00	249.69 232.34
50	6135	0	LYS E	4	8.420	66.812	-1.537	1.00	232.34
	6136	N	LYS E	4	11.173	65.351	-0.540	1.00	232.34
	6137	CA	LYS E	4	9.865	64.939	-1.121	1.00	232.34
	6138 6139	CD	PRO E	5	9.723	66.150	-3.249	1.00	227.45
55	6140	CA	PRO E PRO E	5 5	10.890 9.204	65.481 67.180	-3.843	1.00	124.73
	6141	CB	PRO E	5	10.351	67.180 67.382	-4.150 -5.132	1.00 1.00	227.45
	6142	CG	PRO E	5 .	10.883	66.000	-5.275	1.00	124.73 124.73
	6143	C	PRO E	5	7.921	66.721	-4.845	1.00	227.45
60	6144	0	PRO E	5	7.651	65.522	-4.954	1.00	227.45
w	6145	N	LYS E	6	7.125	67.679	-5.305	1.00	237.93
	6146 6147	CA CB	LYS E Lys e	6	5.877	67.360 67.440	-5.987	1.00	237.93
	6148	CG	LYS E	6 6	4.702 3.370	67.440 67.066	-5.011	1.00	249.69
	6149	CD	LYS E	6	2.244	66.993	-5.640 -4.815	1.00 1.00	249.69
65	6150	CE	LYS E	6	0.935	66.562	-5.275	1.00	249.69 249.69
	6151	NZ	LYS E	6	-0.156	66.352	-4.287	1.00	249.69
	6152	C	LYS E	6	5.650	68.308	-7.153	1.00	237.93
	6153 6154	0	LYS E	6	5.422	69.505	-6.970	1.00	237.93
70	6155	N CA	VAL E VAL E	7 7	5.709 5.533	67.754	-8.356	1.00	162.26
-		<u> </u>	THE E	•	5.532	68.543	-9.567	1.00	162.26

	6156	CB	VAL E	7 .	5.858	67.703	-10.821	1.00	205.67
	6157	CG1	VAL E	7	6.017	68.614	-12.040	1.00	205.67
	6158	CG2:	VAL E	7	7.117	66.881	-10.577	1.00	205.67
5	6159 6160	C	VAL E VAL E	7	4.118	69.111	-9.723	1.00	162.26
3	6161	Ň	SER E	7 8	3.134 4.022	68.364 70.433	-9.717 -9.868	1.00	162.26
	6162	ČA	SER E	8	2./41	71.111	-10.048	1.00 1.00	174.49
	6163	CB	SER E	8	2.672	72.324	-9.131	1.00	174.49 223.27
	6164	OG	SER E	8	3.850	73.111	-9.231	1.00	223.27 223.27
10	6165	С	SER E	8	2.616	71.551	-11.501	1.00	174.49
	6166	0	SER E	8	3.624	71.640	-12.215	1.00	174.49
	6167	N	LEU E	9	1.392	71.815	-11.949	1.00	138.24
	6168 6169	CA CB	Leu e Leu e	9 9	1.200	72.248	-13.338	1.00	138.24
15	6170	CG	LEU E	9	0.497 1.092	71.161 69.761	-14.181 -14.372	1.00 1.00	151.07
	6171	CD1	LEU E	9	0.374	69.105	-15.529	1.00	151.07 151.07
	6172	CD2	LEU E	9	2.578	69.816	-14.665	1.00	151.07
	6173	С	LEU E	9	0.394	73.544	-13.447	1.00	138.24
20	6174	0	LEU E	9	-0.32s	73.919	-12.519	1.00	138.24
20	6175	N	ASN E	10	0.520	74.217	-14.589	1.00	163.51
	6176 6177	CA CB	ASN E ASN E	10 10	-0.215	75.436	-14.823	1.00	163.51
	6178	CG	ASN E	10	0.444 -0.467	76.592 77.788	-14.100 -14.008	1.00	242.89
	6179	OD1	ASN E	10	-1.520	77.730 77.730	·13.369	1.00 1.00	242.89
25	6180	ND2	ASN E	10	-0.077	78.881	-14.650	1.00	242.89 242.89
	6181	С	ASN E	10	-0.303	75.748	-16.310	1.00	163.51
	6182	0	ASN E	10	0.703	76.073	-16.942	1.00	163.51
	6183	N	PRO E	11	-1.515	75.661	-16.902	1.00	167.75
30	6184 6185	CD CA	PRO E	11	-1.686	75.947	-18.332	1.00	141.15
50	6186	CB	PRO E PRO E	11 11	-2.807 -3.740	75.308 75.243	-16.289	1.00	167.75
	6187	CG	PRO E	11	-3.740 -3.151	76.257	-17.494 -18.413	1.00 1.00	141.15
	6188	Č	PRO E	11	-2.804	73.994	-15.505	1.00	141.15 167.75
~~	6189	0	PRO E	11	-1.861	73.210	-15.588	1.00	167.75
35	6190	N	PRO E	12	-3.874	73.736	-14.729	1.00	129.01
	6191	CD	PRO E	12	-5.008	74.630	-14.438	1.00	158.46
	6192 6193	CA CB	PRO E	12	-3. 963	72.506	-13.934	1.00	129.01
	6194	CG	PRO E PRO E	12 12	-5.1 6 4 -5. 29 7	72.766 74.281	-13.028	1.00	158.46
40	6195	č	PRO E	12	-4.198	71.307	-13.015 -14.852	1.00 1.00	158.46 129.01
	6196	Ō	PRO E	12	-3.823	70.178	-14.535	1.00	129.01
	6197	N	TRP E	13	-4.829	71.590	-15.992	1.00	148.97
	6198	CA	TRP E	13	-5.176	70.617	-17.041	1.00	148.97
45	6199	CB	TRP E	13	-5.707	71.376	-18. 25 2	1.00	139.57
4 5 .	6200 6201	CG CD2	TRP E	13 13	-6.745 7.695	72.405	-17.878	1.00	139.57
	6202	CE2	TRP E	13	-7.685 -8.485	72.310 73.479	-16.810	1.00	139.57
	6203	CE3	TRP E	13	-7.934	71.351	-16.851 -15.816	1.00 1.00	139.57 139.57
	6204	CD1	TRP E	13	-7.006	73.598	-18.513	1.00	139.57
50	6205	NE1	TRP E	13	-8.049	74.249	-17.900	1.00	139.57
	6206	CZ2	TRP E	13	-9 .511	73.707	-15. 934	1.00	139.57
	6207 6208	CZ3 CH2	TRP E	13	-8.950	71.581	-14.909	1.00	139.57
	6209	C C	TRP E TRP E	13	-9.731 4.000	72.746	-14.975	1.00	139.57
55	6210	ŏ	TRP E	13 13	-4.000 -3.050	69.772 70.294	-17.478	1.00	148.97
	6211	Ň	ASN E	14	-4.069	68.465	-18.052 -17. 23 6	1.00 1.00	148.97 121.67
	6212	CA	ASN E	14	-2.967	67.569	-17.623	1.00	121.67
	6213	CB	ASN E	14	-2.569	66.659	-16.443	1.00	170.43
60	6214	CG	ASN E	14	-3.669	65.717	-16.039	1.00	170.43
60	6215	OD1	ASN E	14	-4.785	66.134	-15.711	1.00	170.43
	6216 6217	ND2	ASN E	14	-3.382	64.432	-16.058	1.00	170.43
	6218	C O	ASN E ASN E	14 14	-3.273 -3.683	66.730 65.684	-18.871	1.00	121.67
	6219	Ň	ARG E	15	-2.662 -4.227	65.684 67.225	-19.103 -19.661	1.00	121.67
65	6220	ČA	ARG E	15	-4.675	66.616	-19.661 -20.914	1.00 1.00	100.94 100.94
	6221	CB	ARG E	15	-6.069	65.991	-20.773	1.00	110.25
	6222	CG	ARG E	15	-6.278	65.052	-19.581	1.00	110.25
	6223	CD	ARG E	15	-7. 64 2	64.353	-19.673	1.00	110.25
70	6224 6225	NE C7	ARG E	15	-7.673	63.268	-20.667	1.00	110.25
70	0223	CZ	ARG E	15	-8.713	62.965	-21.449	1.00	110.25

	6226	NH1	ARG E	15	-9.818	63.665	-21.363	1.00	110.25
	6227 6228	NH2	ARG E	15	-8.654	61.949	-22.308	1.00	110.25
	6229	C	ARG E ARG E	15 15	-4.797 5.770	67.800	-21.845	1.00	100.94
5	6230	Ň	ILE E	15 16	-5.779 -3.824	68.526 68.012	-21.776 -22.720	1.00	100.94
•	6231	CA	ILE E	16	-3.875	69.182	-23.615	1.00 1.00	114.48
	6232	CB	ILE E	16	-2.723	70.141	-23.315	1.00	114.46 133,29
	6233	CG2	ILE E	16	-3.008	70.920	-22.025	1.00	133.29
10	6234	CG1	ILE E	16	-1.422	69.334	-23.257	1.00	133.29
10	6235 6236	CD1	ILE E	16	-0.187	70.169	-23.241	1.00	133.29
	6237	C O	ILE E	16 16	-3.835 -3.314	68.931 67.000	-25.116	1.00	114.46
	6238	Ň	PHE E	17	-3.314 -4.371	67.920 69.884	-25.573 -25.869	1.00 1.00	114.46
	6239	CA	PHE E	17	-4.389	69.799	·27.315	1.00	157.55 157.55
15	6240	CB	PHE E	17	-5.291	70.875	-27.896	1.00	134.86
	6241	CG	PHE E	17	-6.708	70.444	-28.068	1.00	134.86
	6242	CD1	PHE E	17	-7.747	71.354	-27.884	1.00	134.86
	6243 6244	CD2 CE1	PHE E	17	-7.016		-28.445	1.00	134.86
20	6245	CE2	PHE E PHE E	17 17	-9.085 -8.339	70.974	-28.072	1.00	134.86
	6246	CZ	PHE E	17	-9.378	68.753 69.677	-28.6 3 6 -28.448	1.00	134.86
	6247	č	PHE E	17	-2.984	69.975	-27. 873	1.00 1.00	134.86 157.55
	6248	0	PHE E	17	-2.038	70.221	-27.122	1.00	157.55
05	6249	N	LYS E	18	-2.860	69.858	-29.196	1.00	136.71
25	6250	CA	LYS E	18	-1.582	69.998	-29.892	1.00	136.71
	6251 6252	CB	LYS E	18	-1.660	69.250	-31.219	1.00	249.69
	6253	CD	LYS E Lys e	18 18	-0.384	69.249	-32.033	1.00	249.69
	6254	CE	LYS E	18	-0.530 0.701	68.316 68.337	-33.230 -34.128	1.00	249.69
30	6255	NZ	LYS E	18	0.855	69.643	-34.128 -34.825	1.00 1.00	249.69 249.69
	6256	С	LYS E	18	-1.243	71.471	-30.127	1.00	136.71
	6257	0	LYS E	18	-2.056	72.237	-30.646	1.00	136.71
	6258	N	GLY E	19	-0.042	71.866	-29.726	1.00	201.41
35	6259 6260	CA C	GLY E	19	0.380	73.242	-29.913	1.00	201.41
<i>J</i>	6261	ŏ	GLY E GLY E	19 19	0.195 0.717	74.161 75.279	-28.717	1.00	201.41
	6262	Ň	GLU E	20	-0.541	73.703	-28.708 -27.709	1.00 1.00	201.41 148.40
	6263	CA	GLU E	20	-0.787	74.499	-26.497	1.00	148.40
40	6264	CB	GLU E	20	-2.004	73.945	-25.733	1.00	165.83
40	6265	CG	GLU E	20	-3.267	73.658	-26.577	1.00	165.83
	6266	CD	GLU E	20	-4.479	73.233	-25.726	1.00	165.83
	6267 6268	OE1 OE2	GLU E	20 20	-4.358	72.282	-24.926	1.00	165.83
	6269	C	GLU E	20	-5.555 0.439	73.855 74.469	-25.864 -25.564	1.00 1.00	165.83
45	6270	ŏ	GLU E	20	1.273	73.561	-25.663	1.00	148.40 148.40
	6271	N	ASN E	21	0.552	75.440	-24.653	1.00	156.11
	6272	CA	ASN E	21	1.704	75.474	-23.731	1.00	156.11
	6273	СВ	ASN E	21	2.412	76.835	-23.774	1.00	249.69
50	6274 6275	CG	ASN E	21	2.414	77.468	-25.153	1.00	249.69
50	6276	OD1 ND2	ASN E ASN E	21 21	2.734 2.070	76.825 78.754	-26.157	1.00	249.69
	6277	C	ASN E	21	1.342	75.182	-25.179 -22.267	1.00	249.69
	6278	ت	ASN E	21	0.288	75.589	-22.267 -21.7 6 9	1.00 1.00	156.11 156.11
	6279	N	VAL E	22	2.245	74.493	-21.580	1.00	182,17
55	6280	CA	VAL E	22	2.049	74.137	-20.177	1.00	182.17
	6281	СВ	VAL E	22	1.601	72.669	-20.028	1.00	148.81
	6282 6283	CG1 CG2	VAL E	22	2.757	71.742	-20.356	1.00	148.81
	6284	C	VAL E VAL E	22 22	1.109 3.360	72.404 74.212	-18.627	1.00	148.81
60	6285	ŏ	VAL E	22	4.443	74.313 74.124	-19.407 -19.965	1.00 1.00	182.17
	6286	Ň	THR E	23	3.261	74.650	-18.120	1.00	182.17 131.37
	6287	CA	THR E	23	4.447	74.874	-17.281	1.00	131.37
	6288	СВ	THR E	23	4.448	76.320	-16.723	1.00	249.69
65	6289	OG1	THR E	23	4.251	77.255	-17. 79 4	1.00	249.69
O)	6290 6291	CG2	THR E	23	5.773	76.619	-16.027	1.00	249.69
	6292	C	THR E THR E	23 23	4.559	73.928	-16.088	1.00	131.37
	6293	Ň	LEU E	23 24	3.643 5.694	73.866 73.234	-15.266 -15.974	1.00	131.37
	6294	CA	LEU E	24	5.909	73.234 72.305	-14.862	1.00 1.00	247.08 247.08
70	6295	СВ	LEU E	24	6.490	70.972	-15.357	1.00	141.93

	6296	CG	LEV E	24	6.154	70.407	-16.745	1.00	141.93
	6297	CD1	LEU E	24	6.601	68.946	-16.814	1.00	141.83
	6298	CD2	LEV E	24	4.668	70.513	-17.025	1.00	141.93
_	6299	Č	LEV E	24	6.857	72.886	-13.807	1.00	247.08
5	6300	o	LEU E	24	8.064	72.988	-14.032	1.00	247.08
	6301	N	THR E	25	6.302	73.254	-12.653	1.00	187.47
	6302 6303	CA CB	THR E	25 25	7.075	73.824	-11.547	1.00	187.47
	6304	OG1	THR E	25 25	6.280 5.936	74.957 75.964	-10.847 -11.806	1.00	161.19
10	6305	CG2	THR E	25	7.100	75.590	-9.725	1.00 1.00	161.19
	6306	C	THR E	25	7.391	72.739	-10.512	1.00	161.19 187.47
	6307	0	THR E	25	6.513	71.981	-10.121	1.00	187.47
	6308	N	CYS E	26	8.642	72.673	-10.069	1.00	208.94
1.5	6309	CA	CYS E	26	9.057	71.677	-9.078	1.00	208.94
15	6310	C	CYS E	26	8.680	72.137	-7.667	1.00	208.94
	6311 6312	СВ	CYS E	26 26	8.738 10.562	73.326 71.439	-7.364 0.470	1.00	208.94
	6313	SG	CYS E	26	11.190	71.439 70.046	-9.1 7 9 -8.197	1.00 1.00	205.14
	6314	Ñ	ASN E	27	8.303	71.189	-6.812	1.00	205.14 249.69
20	6315	CA	ASN E	27	7.875	71.478	-5.439	1.00	249.69
	6316	СВ	ASN E	27	8.415	70.418	-4.468	1.00	249.69
	6317	ÇG	ASN E	27	7.792	70.526	-3.076	1.00	249.69
	6318	OD1	ASN E	27	6.569	70.623	-2.936	1.00	249.69
25	6319	ND2	ASN E	27	8.632	70.505	-2.043	1.00	249.69
23	6320 6321	C O	ASN E ASN E	27 27	8.241	72.870 72.005	-4.9 3 0	1.00	249.69
	6322	Ň	GLY E	28	9.333 7.301	73.095 73.795	-4.401 -5.095	1.00 1.00	249.69
	6323	CA	GLY E	28	7.486	75.172	-4.669	1.00	249.69 249.69
	6324	· c	GLY E	28	6.306	75.960	-5.202	1.00	249.69
30	6325	0	GLY E	28	6.092	76.005	-6.419	1.00	249.69
	6326	Ņ	ASN E	29	5.537	76.576	-4.305	1.00	249.69
	6327	CA	ASN E	29	4.349	77.334	-4.702	1.00	249.69
	6328 6329	CB CG	ASN E	29	3.447	77.573	-3.470	1.00	249.69
35	6330	OD1	ASN E ASN E	29 29	2.043 1.664	78.092 78.143	-3.837 -5.013	1.00	249.69
-	6331	ND2	ASN E	29	1.268	78.469	-2.8 2 1	1.00 1.00	249.69 249.69
	6332	C	ASN E	29	4.659	78.665	-5.406	1.00	249.69
	6333	0	ASN E	29	4.147	78.925	-6.509	1.00	249.69
40	6334	N	ASN E	30	5.502	79.498	-4.796	1.00	249.69
40	6335	CA	ASN E	30	5.807	80.792	-5.395	1.00	249.69
	6336 6337	CB	ASN E	30	5.157	81.904	-4.559	1.00	249.69
	6338	CG OD1	ASN E ASN E	30 30	3.636 3.012	81.814	-4. 54 3	1.00	249.69
	6339	ND2	ASN E	30	3.030	81.900 81.646	-3.481 -5.721	1.00 1.00	249.69
45	6340	C	ASN E	30	7.288	81.109	-5.624	1.00	249.69 249.69
	6341	O	ASN E	30	7.734	81.191	-6.773	1.00	249.69
	6342	N	PHE E	31	8.047	81.290	-4.544	1.00	249.25
	6343	CA	PHE E	31	9.464	81. 63 4	-4.672	1.00	249.25
50	6344	CB	PHE E	31	9.744	82.979	-3.973	1.00	249.69
50	6345 6346	CG CD1	PHE E PHE E	31	8.853	84.109	-4.448	1.00	249.69
	6347	CD2	PHE E PHE E	31 31	7.546 9.307	84.234 85.030	-3.971 5.207	1.00	249.69
~	6348	CE1	PHE E	31	6.702	85.255	-5.397 -4.433	1.00	249.69
	6349	CE2	PHE E	31	8.470	86.054	-5.864	1.00 1.00	249.69 249.69
55	6350	CZ	PHE E	31	7.167	86.166	-5.380	1.00	249.69
	6351	C	PHE E	31	10.439	80.568	-4.166	1.00	249.25
	6352	0	PHE E	31	10.399	80.170	-3.004	1.00	249.25
	6353	N	PHE E	32	11.324	80.127	-5.061	1.00	241.74
60	6354 6355	CA CB	PHE E	32	12.329	79.106	-4.757	1.00	241.74
00	6356	CG	PHE E	32	12.131	77.894	-5.677 5.004	1.00	249.69
	6357	CD1	PHE E PHE E	32 32	12.858 12.489	76.648 75.993	-5.224 -4.048	1.00 1.00	249.69
	6358	CD2	PHE E	32	13.905	76.121	-5.984	1.00	249.69 249.69
	6359	CE1	PHE E	32	13.150	74.834	-3.639	1.00	249.69
65	6360	CE2	PHE E	32	14.570	74.962	-5.582	1.00	249.69
	6361	CZ	PHE E	32	14.191	74.320	-4.407	1.00	249.69
	6362	C	PHE E	32	13.743	79.667	-4.926	1.00	241.74
	6363	O	PHE E	32	13.927	80.745	-5.490	1.00	241.74
70	6364 6365	N CA	GLU E	33	14.739	78.916	-4.465 4.504	1.00	249.60
, ,	0000	∪A.	GLU E	33	16.114	79.383	-4.531	1.00	249.60

	6366	CB	GLU E	33 ·	16.663	79.497	-3.101	1.00	249.49
	6367	CG	GLU E	33	17.893	80.382	-2.971	1.00	249.49
	6368	CD	GLU E	33	17.724	81.732	-3.659	1.00	249.49
5	6369 6370	OE1 OE2	GLU E GLU E	33	16.677	82.386	-3.446	1.00	249.49
,	6371	C	GLU E	33 33	18.641 17.112	82.137 78.603	-4.409 5.404	1.00	249.49
	6372	ŏ	GLU E	33	17.112	79.197	-5.404 -6.225	1.00 1.00	249.60
	6373	N	VAL E	34	17.179	77.285	-5.229	1.00	249.60
	6374	CA	VAL E	34	18.123	76.456	-5.982	1.00	249.69 249.69
10	6375	CB	VAL E	34	18.005	74.970	-5.541	1.00	249.69
	6376	CG1	VAL E	34	19.019	74.118	-6.281	1.00	249.69
	6377 6378	CG2 C	VAL E VAL E	34 34	18.228	74.858	-4.032	1.00	249.69
	6379	ŏ	VAL E	34	18.014 16.936	76.540 76.775	-7.511	1.00	249.69
15	6380	Ň	SER E	35	19.152	76.355	-8.062 -8.178	1.00 1.00	249.69
	6381	CA	SER E	35	19.231	76.387	-9.638	1.00	248.45 248.45
	6382	СВ	SER E	35	20.377	77.287	-10.097	1.00	249.69
	6383	og	SER E	35	21.627	76.682	-9.830	1.00	249.69
20	6384 6385	C	SER E	35	19.485	74.969	-10.140	1.00	248.45
20	6386	N .	SER E SER E	35 36	19.572 19.622	74.732	-11.350	1.00	248.45
	6387	ČA	SER E	36	19.865	74.036 72.628	-9.196 -9.516	1.00 1.00	249.69
	6388	CB	SER E	36	20.966	72.043	-8.614	1.00	249.69 244.12
0.5	6389	OG	SER E	36	20.521	71.874	-7.278	1.00	244.12
25	6390	C	SER E	36	18.578	71.819	-9.352	1.00	249.69
	6391	, O	SER E	36	18.259	71.325	-8.266	1.00	249.69
	6392 6393	` N CA	THR E THR E	37	17.836	71.701	-10.449	1.00	208.63
	6394	CB	THR E	37 37	16.589 15.388	70.958 71.911	-10.462	1.00	208.63
30	6395	OG1	THR E	37	15.343	71.911 72.880	-10.670 -9.604	1.00 1.00	197.00
	6396	CG2	THR E	37	14.089	71.128	-10.693	1.00	197.00 197.00
	6397	С	THR E	37	16.689	69.957	-11.608	1.00	208.63
	6398	O	THR E	37	17.186	70.277	-12.687	1.00	208.63
35	6399 6400	N CA	LYS E	38	16.236	68.739	-11.366	1.00	223.46
55	6401	CB	LYS E Lys e	38 38	16.309 16.899	67.708 66.425	-12.384	1.00	223.46
	6402	CG	LYS E	38	18.295	66.620	-11.765 -11.158	1.00 1.00	231.11
	6403	CD	LYS E	38	18.852	65.344	-10.528	1.00	231.11 231.11
40	6404	CE	LYS E	38	20.261	65.567	-9.976	1.00	231.11
40	6405	NZ	LYS E	38	20.853	64.342	-9.367	1.00	231.11
	6406 6407	C	LYS E	38	14.947	67.420	-13.018	1.00	223.46
	6408	O N	LYS E TRP E	38 39	13.914	67.492	-12.361	1.00	223.46
	6409	ČA	TRP E	39	14.951 13.721	67.117 66.798	-14.308 -15.022	1.00 1.00	249.08
45	6410	СВ	TRP E	39	13.373	67.909	-16.006	1.00	249.08 173.34
	6411	CG	TRP E	39	12.996	69.216	-15.384	1.00	173.34
	6412	CD2	TRP E	39	11.899	69.476	-14.483	1.00	173.34
	6413	CE2	TRP E	39	11.857	70.869	-14.267	1.00	173.34
50	6414 6415	CE3 CD1	TRP E TRP E	39	10.957	68.673	-13.840	1.00	173.34
-	6416	NE1	TRP E	39 39	13.550 12.871	70.422 71.424	-15.660	1.00	173.34
	6417	CZ2	TRP E	39	10.911	71.476	-14.998 -13.440	1.00 1.00	173.34 173.34
	6418	CZ3	TRP E	39	10.011	69.281	-13.014	1.00	173.34
55	6419	CH2	TRP E	39	9.995	70.668	-12.828	1.00	173.34
55	6420	C	TRP E	39	13.964	65.501	-15.788	1.00	249.08
	6421 6422	0 N	TRP E PHE E	39	14.993	65.363	-16.450	1.00	249.08
	6423	CA	PHE E	40 40	13.032 13.206	64.553 63.281	-15.700	1.00	178.94
	6424	CB	PHE E	40	13.435	62.145	-16.394 -15.383	1.00 1.00	178.94
60	6425	CG	PHE E	40	14.631	62.341	-14.475	1.00	249.69 249.69
•	6426	CD1	PHE E	40	14.543	63.160	-13.347	1.00	249.69
	6427	CD2	PHE E	40	15.836	61.678	-14.729	1.00	249.69
	6428 6429	CE1	PHE E	40	15.632	63.313	-12.484	1.00	249.69
65	6429 6430	CE2 CZ	PHE E PHE E	40 40	16.928	61.826	-13.873	1.00	249.69
J J	6431	C	PHE E	40 40	16.824 12.051	62.645 62.8 9 6	-12.748	1.00	249.69
	6432	ŏ	PHE E	40	11.245	62.027	-17.323 -16.988	1.00 1.00	178.94 178.94
	6433	N	HIS E	41	11.992	63.534	-18.488	1.00	163.57
70	6434	CA	HIS E	41	10.961	63.256	-19.477	1.00	163.57
70	6435	СВ	HIS E	41	11.070	64.259	-20.627	1.00	157.46

	6436 6437	CG CD2	HIS E	41- 41	10.025 10.104	64.069 64.164	-21.695	1.00	157.46
	6438	ND1	HIS E	41	8.710	63.777	-23.048 -21.411	1.00	157.46
5	6439	CE1	HIS E	41	8.018	63.698	-22.540	1.00 1.00	157.46
ر	6440 6441	NE2	HIS E	41	8.840	63.930	-23.544	1.00	157.46 157.46
	6442	C	HIS E	41	11.067	61.816	-20.031	1.00	163,57
	6443	Ŋ	HIS E ASN E	41	11.955	61.520	-20.841	1.00	163.57
	6444	CA	ASN E	42 42	10.149 10.139	60.937	-19.611	1.00	166.06
10	6445	CB	ASN E	42	10.165	59.529 59.393	-20.031	1.00	166.06
	6446	CG	ASN E	42	8.800	59.655	-21.564	1.00	227.72
	6447	OD1	ASN E	42	8.150	60.654	-22.205 -21.900	1.00	227.72
	6448	ND2	ASN E	42	8.370	58.767	-23.101	1.00 1.00	227.72
15	6449	C	ASN E	42	11.348	58.828	-19.424	1.00	227.72 166.06
1.5	6450 6451	0 N	ASN E	42	11.820	57.822	-19.950	1.00	166.06
	6452	CA	GLY E GLY E	43	11.829	59.368	-18.305	1.00	222.62
	6453	Č	GLY E	43 43	12.985	58.804	-17.627	1.00	222.62
	6454	ŏ	GLY E	43	14. 27 2 15.139	59.493 50.780	-18.049	1.00	222.62
20	6455	N	SER E	44	14.388	59.780 59.764	-17.220	1.00	222.62
	6456	CA	SER E	44	15.560	60.424	-19.346 -19.919	1.00	232.48
	6457	CB	SER E	44	15.391	60.572	-21.435	1.00	232.48
	6458	og	SER E	44	15.207	59.322	-22.064	1.00 1.00	196.92
25	6459 6460	C	SER E	44	15.788	61.806	-19.322	1.00	196.92 232.48
23	6461	0 N	SER E	44	14.908	62.661	-19.386	1.00	232.48
	6462	CA	LEU E LEU E	45	16.970	62.033	-18.759	1.00	247.61
	6463	CB	LEU E	45 45	17.273	63.331	-18.173	1.00	247.61
	6464	ČĞ	LEU E	45 45	18.722	63.380	-17.682	1.00	238.67
30	6465	CD1	LEU E	45	19.128 18.176	64.690 64.989	-16.996	1.00	238.67
	6466	CD2	LEU E	45	20.552	64.584	-15.849	1.00	238.67
	6467	Ç	LEU E	45	17.030	64.445	-16.486 -19.194	1.00 1.00	238.67
	6468	0	LEU E	45	17.195	64.244	-20.401	1.00	247.61
35	6469 6470	N	SER E	46	16.630	65.616	-18.700	1.00	247.61 233.41
33	6471	CA CB	SER E	46	16.339	66.768	-19.550	1.00	233.41
	6472	OG OG	SER E SER E	46	15.009	67.411	-19.131	1.00	241.98
	6473	č	SER E	46 46	14.644	68.461	-20.012	1.00	241.98
	6474	Ö	SER E	46	17.450 18.358	67.806 67.721	-19.498	1.00	233.41
40	6475	N	GLU E	47	17.353	68.798	-18.670	1.00	233.41
	6476	CA	GLU E	47	18.353	69.858	-20.378 -20.479	1.00 1.00	249.69
	6477	CB	GLU E	47	18.508	70.268	-21.943	1.00	249.69
	6478 6479	CG	GLU E	47	18.990	69.136	-22.837	1.00	249.69 249.69
45	6480	CD OE1	GLU E	47	19.114	69.555	-24.287	1.00	249.69
	6481	OE2	GLU E GLU E	47 47	18.075	69.901	-24.896	1.00	249.69
	6482	Č	GLU E	47	20,247 18,118	69.540	-24.819	1.00	249.69
	6483	0	GLU E	47	19.014	71.111 71.949	-19.629	1.00	249.69
50	6484	N	GLU E	48	16.925	71.256	-19.500 -19.062	1.00	249.69
50	6485	CA	GLU E	48	16.652	72.417	-18.231	1.00 1.00	197.12
	6486 6487	CB	GLU E	48	15.153	72.734	-18.213	1.00	197.12 231.64
	6488	CG CD	GLU E	48	14.768	73.878	-17.276	1.00	231.64
	6489	OE1	GLU E	48	15.355	75.216	-17.688	1.00	231.64
55	6490	OE2	GLU E	48 48	14.884	75.786	-18.695	1.00	231.64
	6491	Č	GLU E	48	16.286 17.147	75.698	-17.004	1.00	231.64
	6492	0	GLU E	48	17.288	72.146 70.990	-16.813	1.00	197.12
	6493	N	THR E	49	17.420	73.221	-16.397 -16.080	1.00	197.12
60	6494	CA	THR E	49	17.901	73.124	-14.707	1.00 1.00	219.19
00	6495 6496	CB	THR E	49	19.370	73.557	-14.610	1.00	219.19 249.63
	6497	OG1 CG2	THR E	49	19.517	74.871	-15.170	1.00	249.63
	6498	C	THR E	49	20.263	72.574	-15.363	1.00	249.63
	6499	ŏ	THR E THR E	49 49	17.060	74.007	-13.794	1.00	219.19
65	6500	Ň	ASN E	49 50	16.949 16.475	73.749	-12.597	1.00	219.19
	6501	CA	ASN E	50	15.625	75.055 75.963	-14.364	1.00	248.24
	6502	CB	ASN E	50	15.070	75.963 77.051	-13.603	1.00	248.24
	6503	CG	ASN E	50	14.389	78.172	-14.530 -13.770	1.00	249.69
70	6504 6505	OD1	ASN E	50	14.025	78.004	-12.606	1.00 1.00	249.69 249.69
, 0	0000	ND2	ASN E	50	14.201	79.314	-14.428	1.00	249.69 249.69
							· ·		473.00

	6506	С	ASN E	50	14.479	75.129	-13.024	1.00	248.24
	6507	0	asn e	50	14.117	74.104	-13.598	1.00	248.24
	6508	N	SER E	51	13.906	75.553	-11.900	1.00	208.41
5	6509	CA ·	SER E	51	12.811	74.797	-11.296	1.00	208.41
3	6510 6511	CB OG	SER E SER E	51 51	12.509	75.325	-9.894	1.00	181.70
	6512	C	SER E	51 51	11.848 11.524	76.577 74.814	-9.948 -12.142	1.00	181.70
	6513	ŏ	SER E	51	10.625	73.998	-12.142	1.00 1.00	208.41
	6514	Ñ	SER E	52	11.434	75.735	-13.100	1.00	208.41
10	6515	CA	SER E	52	10.254	75.830	-13.962	1.00	201.05 201.05
	6516	СВ	SER E	52	9.717	77.259	-13.995	1.00	181.26
	6517	og	SER E	52	9.309	77.679	-12.707	1.00	181.26
	6518 6519	C O	SER E	52	10.551	75.390	-15.385	1.00	201.05
15	6520	N	SER E LEU E	52 53	11.180	76.117	-16.157	1.00	201.05
	6521	CA	LEU E	53 53	10.088 10.287	74.194 73.643	-15.724	1.00	168.60
	6522	CB	LEU E	53	10.287	73.132	-17.058 -16.970	1.00 1.00	168.60
	6523	CG	LEU E	53	10.304	71.282	-18.231	1.00	122.87 122.87
••	6524	CD1	LEU E	53	10.969	71.906	-19.463	1.00	122.87
20	6525	CD2	LEU E	53	10.854	69.900	-17.957	1.00	122.87
	6526	Ç	LEU E	53	9.077	73.940	-17.340	1.00	168.60
	6527	0	LEU E	53	8.020	73.327	-17.805	1.00	168.60
	6528 6529	N CA	ASN E ASN E	54 54	9.235	74.892	-18.848	1.00	150.56
25	6530	CB	ASN E	54 54	8.149 8.319	75.251 76.683	-19.729	1.00	150.56
	6531	ČĠ	ASN E	54	8.080	77.699	-20.233 -19.151	1.00 1.00	229.83
	6532	OD1	ASN E	54	7.052	77.669	-18.479	1.00	229.83 229.83
	6533	ND2	ASN E	54	9.029	78.606	-18.972	1.00	229.83
20	6534	Ç	ASN E	54	8.032	74.311	-20.905	1.00	150.56
30	6535	0	ASN E	54	8.977	73.598	-21.260	1.00	150.56
	6536 6537	N	ILE E	55	6.840	74.322	-21.495	1.00	211.09
	6538	CA CB	ILE E	55 55	6.499	73.504	-22.654	1.00	211.09
	6539	CG2	ILE E	55	5.596 4.804	72.306 71.809	-22.246	1.00	170.97
35	6540	CG1	ILE E	55	6.460	71.189	-23.445 -21.638	1.00 1.00	170.97
	6541	CD1	ILE E	55	5.686	69. 96 0	-21.201	1.00	170.97 170.97
	6542	С	ILE E	55	5.745	74.400	-23.628	1.00	211.09
	6543	, 0	ILE E	55	4.659	74.893	-23.314	1.00	211.09
40	6544	N	VAL E	56	6.329	74.624	-24.799	1.00	155.17
40	6545 6546	CA CB	VAL E	56	5.684	75.466	-25.778	1.00	155.17
	6547	CG1	VAL E VAL E	56 56	6.705	76.318	-26.516	1.00	247.89
	6548	CG2	VAL E	56	6.008 7.780	77.514 76.778	-27.154	1.00	247.89
	6549	Č	VAL E	56	4.917	74.606	-25.550 -26.770	1.00 1.00	247.89
45	6550	0	VAL E	56	4.585	73.468	-26.458	1.00	155.17 155.17
	6551	N	ASN E	57	4.639	75.144	-27.959	1.00	169.22
	6552	CA	ASN E	57	3.886	74.432	-28.996	1.00	169.22
	6553 6554	CB	ASN E	57	4.365	74.837	-30.389	1.00	237.27
50	6555	CG OD1	ASN E	57	3.979	76.263	-30.731	1.00	237.27
50	6556	ND2	ASN E ASN E	57 57	2.817 4.953	76.650	-30.605	1.00	237.27
	6557	C	ASN E	57 57	4.853 3.941	77.055 72.925	-31.165	1.00	237.27
	6558	ŏ	ASN E	57	4.860	72.255	-28.825 -29.300	1.00 1.00	169.22
	6559	N	ALA E	58	2.923	72.424	-28.128	1.00	169,22 152,74
55	6560	CA	ALA E	58	2.746	71.015	-27.787	1.00	152.74
	6561	CB	ALA E	58	1.438	70.847	-27.040	1.00	133.90
	6562 6563	C	ALA E	58	2.812	70.012	-28.932	1.00	152.74
	6564	0 N	ALA E	58	1.888	69.915	-29.751	1.00	152.74
60	6565	CA	LYS E Lys e	59 59	3.909	69.258	-28.966	1.00	179.74
	6566	CB	LYS E	59	4.128 5.572	68.226 68.264	-29.976	1.00	179.74
	6567	CG	LYS E	59	5.967	68.264 69.596	-30.469 -31.093	1.00 1.00	249.69
	6568	CD	LYS E	59	7.446	69.638	-31.093 -31.470	1.00	249.69 249.69
CE	6569	CE	LYS E	59	7.825	71.010	-32.032	1.00	249.69
65	6570	NZ	LYS E	59	9.265	71.091	-32.425	1.00	249.69
	6571 6572	C	LYS E	59	3.853	66.896	-29.300	1.00	179.74
	6572 6573	O N	LYS E	59	4.242	66.677	-28.156	1.00	179.74
	6574	N CA	PHE E PHE E	60 60	3.175	66.009	-30.009	1.00	187.69
70	6575	CB	PHE E	60 60	2.825 2.441	64.706 83.771	-29.466	1.00	187.69
				50	£.44 }	63.771	-30.613	1.00	249.39

	6576 6577 6578	CG CD1 CD2	PHE E PHE E PHE E	60 60	1.209 1.035 0.214	64.201 63.865 64.930	-31.352 -32.689 -30.707	1.00 1.00 1.00	249.39 249.39
_	6579	CE1	PHE E	60	-0.111	64.248	-33.377	1.00	249.39 249.39
5	6580	CE2	PHE E	60	-0.939	65.319	-31.386	1.00	249.39
	6581	cz	PHE E	60	-1.101	64.976	-32.724	1.00	249.39
	6582 6583	C	PHE E	60 60	3.927	64.073	-28.626	1.00	187.69
	6584	Ň	GLU E	60 61	3.642 5.181	63.338 64.364	-27.683	1.00	187.69
10	6585	CA	GLU E	61	6.335	63.808	-28.965 -28.255	1.00 1.00	196.09
	6586	СВ	GLU E	61	7.623	64.147	-29.010	1.00	196.09 249.51
	6587	CG	GLU E	61	7.682	63.618	-30.447	1.00	249.51
	6588	CD	GLU E	61	6.550	64.132	-31.336	1.00	249.51
15	6589 6590	OE1 OE2	GLU E	61 61	6.341	65.363	-31.403	1.00	249.51
1,5	6591	C	GLU E	61 61	5.872 6.433	63.302 64.313	-31.976 -26.820	1.00 1.00	249.51
	6592	ŏ	GLU E	61	7.042	63.668	-25.965	1.00	196.09 196.09
	6593	N	ASP E	62	5.831	65.470	-26.566	1.00	216.24
20	6594	;A	ASP E	62	5.842	66.063	-25.235	1.00	216.24
20	6595	CB	ASP E	62	5.333	67.500	-25.285	1.00	214.73
	6596 6597	CG OD1	ASP E	62 62	6.047	68.327	-26.319	1.00	214.73
	6598	OD2	ASP E	62	7.249 5.416	68.076 69.232	-26.535	1.00	214.73
	6599	C	ASP E	62	4.971	65.264	-26.906 -24.279	1.00 1.00	214.73
25	6600	Ō	ASP E	62	5.152	65.325	-23.063	1.00	216.24 216.24
	6601	N	SER E	63	4.009	64.532	-24.831	1.00	123.78
	6602	CA	SER E	63	3.127	63.707	-24.015	1.00	123.78
	6603 6604	CB OG	SER E	63	2.085	62.988	-24.899	1.00	115.99
30	6605	C	SER E SER E	63 63	1.319	63.897	-25.674	1.00	115.99
50	6606	ŏ	SER E	63 63	4.011 4.783	62.669 61.957	-23.301 -23.934	1.00	123.78
	6607	Ň	GLY E	64	3.908	62.584	-23.934 -21.986	1.00 1.00	123.78 143.97
	6608	CA	GLY E	64	4.723	61.615	-21.294	1.00	143.97
35	6609	C .	GLY E	64	4.739	61.721	-19.786	1.00	143.97
33	6610	0	GLY E	64	3.910	62.406	-19.184	1.00	143.97
	6611 6612	N CA	GLU E	65 65	5.707	61.027	-19.190	1.00	147.25
	6613	CB	GLU E	65	5.904 6.138	60.964 59.507	-17. 74 3 -17.358	1.00	147.25
	6614	CG	GLU E	65	6.548	59.268	-17.336	1.00 1.00	197.50 197.50
40	6615	CD	GLU E	65	7.152	57.894	-15.759	1.00	197.50
	6616	OE1	GLU E	65	8.198	57.63 0	-16.379	1.00	197.50
	6617	OE2	GLU E	65	6.587	57.076	-15.015	1.00	197.50
	6618 6619	C	GLU E	65 65	7.097	61.824	-17.309	1.00	147.25
45	6620	N	TYR E	65 66	8.215 6.859	61.604 62.792	-17. 76 6	1.00	147.25
	6621	ĊA	TYR E	66	7.924	63.682	-16.423 -15.948	1.00 1.60	205.23 205.23
	6622	СВ	TYR E	66	7.595	65.141	-16.266	1.00	153.79
	6623	CG	TYR E	66	7.502	65.522	-17.726	1.00	153.79
50	6624	CD1	TYR E	66	6.391	65.194	-18.490	1.00	153.79
20	6625 6626	CE1	TYR E	66	6.265	65.628	-19.806	1.00	153.79
	6627	CD2 CE2	TYR E	66 66	8.491 8.377	66.286 66.729	-18.316	1.00	153.79
	6628	cz	TYR E	66	7.265	66.403	-19.628 -20.358	1.00 1.00	153.79
	6629	OH	TYR E	66	7.159	66.870	-21.583	1.00	153.79 153.79
55	6630	С	TYR F	66	8.179	63.597	-14.442	1.00	205.23
	6631	0	TYR E	66	7.402	62.979	-13.710	1.00	205.23
	6632 6833	N	LYS E	67	9.261	64.248	-13.997	1.00	187.13
	6634	CA CB	LYS E LYS E	67 67	9.646	64.287	-12.580	1.00	187.13
60	6635	CG	LYS E	67	9.961 10.969	62.882 62.131	-12.071 -12.908	1.00	169.14
	6636	CD	LYS E	67	11.160	60.730	-12.365	1.00 1.00	169.14 169.14
	6637	CE	LYS E	67	11.800	59.810	-13.402	1.00	169.14
	6638	NZ	LYS E	67	12.045	58.414	-12.897	1.00	169.14
65	6639	C	LYS E	67	10.842	65.185	-12.276	1.00	187.13
UJ.	6640 6641	O N	LYS E	67 69	11.685	65.433	-13.141	1.00	187.13
	6642	CA	CYS E	68 68	10.902 12.004	65.666 68.516	-11.032	1.00	161.02
	6643	č	CYS E	68	12.590	66.515 66.008	-10.582 -9.267	1.00	161.02
~ ^	6644	ŏ	CYS E	68	11.900	65.396	-9.267 -8.456	1.00 1.00	161.02 161.02
70	6645	CB	CYS E	68	11.567	67.993	-10.447	1.00	132.43
						•			

	6646	SG	CYS E	68	10.402	68.415	-9.105	1.00	132.43
	6647	N	GLN E	69	13.880	66.274	-9.084	1.00	233.39
	6648	CA:	GLN E	69	14.623	65.865	-7.903	1.00	233.39
	6649	CB	GLN E	69	15.252	64.494	-8.156	1.00	249.52
5	6650	CG	GLN E	69	16.420	64.156	-7.253	1.00	
	6651	CD	GLN E	69	17.095	62.850	-7.643		249.52
	6652	OE1	GLN E	69	17.462	62.650	-8.803	1.00	249.52
	6653	NE2	GLN E	69	17.266	61.957		1.00	249.52
	6654	C	GLN E	69	15.709		-6.673	1.00	249.52
10	6655	ŏ	GLN E			66.900	-7.632	1.00	233.39
10	6656	N		69	16.242	67.505	-8.563	1.00	233.39
	6657	ČA		70	16.037	67.108	-6.363	1.00	249.69
			HIS E	70	17.076	68.070	-6.015	1.00	249.69
	6658	CB	HIS E	70	16.657	68.885	-4.790	1.00	243.01
15	6659	CG	HIS E	70	15.547	69.852	-5.068	1.00	243.01
13	6660	CD2	HIS E	70	14.356	70.039	-4.454	1.00	243.01
	6661	ND1	HIS E	70	15.605	70.774	-6.089	1.00	243.01
	6662	CE1	HIS E	70	14.495	71.493	-6.096	1.00	243.01
	6663	NE2	HIS E	70	13.721	71.068	-5.114	1.00	243.01
••	6664	С	HIS E	70	18.414	67.388	-5.761	1.00	249.69
20	6665	0	HIS E	70	18.575	66.198	-6.034	1.00	249.69
	6666	N	GLN E	71	19.370	68.148	-5.238	1.00	231.62
	6667	CA	GLN E	71	20.708	67.634	-4.952	1.00	
	6668	CB	GLN E	71	21.554	68.756	-4.329	1.00	231.62
	6669	CG	GLN E	71	23.080	68.559	-4.380	1.00	249.69
25	6670	CD	GLN E	71	23.634	68.488	-5. 80 3	1.00	249.69
	6671	OE1	GLN E	71	23.304	69.316		1.00	249.69
	6672	NE2	GLN E	71	24.495		-6.663	1.00	249.69
	6673	C	GLN E	71		67.503	-6.049	1.00	249.69
	6674	ŏ	GLN E		20.677	66.413	-4.022	1.00	231.62
30	6675	N		71	21.311	65.389	-4.298	1.00	231.62
50	6676	CA CA	GLN E	72	19.928	66.528	-2.928	1.00	249.69
			GLN E	72	19.819	65.448	-1.951	1.00	249.69
	6677	CB	GLN E	72	20.601	65.834	-0.689	1.00	249.69
	6678	CG	GLN E	72	20.626	64.791	0.419	1.00	249.69
25	6679	CD	GLN E	72	21.284	65.315	1.687	1.00	249.69
35	6680	OE1	GLN E	72	22.439	65.746	1.664	1.00	249.69
	6681	NE2	GLN E	72	20.549	65.281	2.799	1.00	249.69
	6682	С	GLN E	72	18.349	65.170	-1.607	1.00	249.69
	6683	0	GLN E	72	17.948	65.208	-0.444	1.00	249.69
40	6684	N	VAL E	73	17.544	64.899	-2.627	1.00	249.30
40	6685	CA	VAL E	73	16.128	64.614	-2.427	1.00	249.30
	6686	CB	VAL E	73	15.243	65.860	-2.707	1.00	249.69
	6687	CG1	VAL E	73	13.838	65.614	-2.192	1.00	249.69
	6688	CG2	VAL E	73	15.843	67.101	-2.058	1.00	249.69
	6689	С	VAL E	73	15.709	63.512	-3.386	1.00	
45	6690	0	VAL E	73	16.183	63.451	-4.516	1.00	249.30
	6691	Ñ	ASN E	74	14.817	62.642	-2.937		249.30
	6692	CA	ASN E	74	14.345	61.555		1.00	249.46
	6693	CB	ASN E	74	13.714		-3.783	1.00	249.46
	6694	ČĠ	ASN E	74		60.460	-2.912	1.00	249.69
50	6695	OD1	ASN E	74	14.665 15.859	59.960	-1.825	1.00	249.69
-	6696	ND2	ASN E			59. 76 9	-2.080	1.00	249.69
	6697			74	14.139	59.737	-0.621	1.00	249.69
		C	ASN E	74	13.346	62.081	-4.826	1.00	249.46
	6698	0	ASN E	74	12.387	62.774	-4.485	1.00	249.46
55	6699	N.	GLU E	75	13.587	61.755	-6.094	1.00	249.69
22	6700	CA	GLU E	75	12.740	62.194	-7.209	1.00	249.69
	6701	CB	GLU E	75	13.082	61.386	-8.468	1.00	249.69
	6702	CG	GLU E	75	13.431	59.924	-8.199	1.00	249.69
	6703	CD	GLU E	75	14.002	59.221	-9.425	1.00	249.69
	6704	OE1	GLU E	75	14.946	59.768	-10.042	1.00	249.69
60	6705	OE2	GLU E	75	13.515	58.118	-9.768	1.00	249.69
	6706	С	GLU E	75	11.233	62.147	-6.941	1.00	249.69
	6707	0	GLU E	75	10.724	61.213	-6.320	1.00	249.69
	6708	N	SER E	76	10.531	63.168			
	6709	CA	SER E	76	9.083	63.302	-7.428 -7.244	1.00	190.25
65	6710	CB	SER E	76	8.613	64.871	-7.244 -7.742	1.00	190.25
	6711	ÖĞ	SER E	76			-7.743	1.00	199.25
	6712	č	SER E	76	8.614	64.717	-9.163	1.00	199.25
	6713	ŏ	SER E		8.265	62.236	-7.954	1.00	190.25
	6714	Ň		76 77	8.728	61.612	-8.907	1.00	190.25
70	6715	CA	GLU E	77 77	7.038	62.044	-7.481	1.00	235.50
. •	0, 10	<u> </u>	GLU E	77	6.135	61.072	-8.079	1.00	235.50

	~~4			_					
	6716 6717	CB CG	GLU E GLU E	77· 77	4.839 5.029	60.973	-7.269	1.00	249.14
	6718	CD:	GLU E	77	5.532	60.405 58.966	-5.870 -5.879	1.00	249.14
	6719	OE1	GLU E	77	5.869	58.450	-6.966	1.00 1.00	249.14 249.14
5	6720	OE2	GLU E	77	5.594	58.349	-4.795	1.00	249.14
	6721	C	GLU E	77	5.826	61.543	-9.488	1.00	235.50
	6722 6723	- O N	GLU E PRO E	77 70	5.181	62.569	-9.672	1.00	235.50
	6724	CD	PRO E	78 78	6.280 6.805	60.791 59.420	-10.505	1.00	173.10
10	6725	CA	PRO E	78	6.055	61.144	-10.383 -11.915	1.00 1.00	109.00
	6726	CB	PRO E	78	6.320	59.831	-12.652	1.00	173.10 109.00
	6727	CG	PRO E	78	7.324	59.145	-11.779	1.00	109.00
	6728	Č	PRO E	78	4.648	61.657	-12.182	1.00	173.10
15	6729 6730	O N	PRO E	78 70	3.721	61.375	-11.410	1.00	173.10
15	6731	CA	VAL E VAL E	79 79	4.490 3.168	62.430 62.929	-13.253	1.00	170.14
	6732	CB	VAL E	79	2.986	64.448	-13.628 -13.378	1.00 1.00	170.14
	6733	CG1	VAL E	79	1.708	64.936	-14.057	1.00	117.67 117.67
	6734	CG2	VAL E	79	2.879	64.719	-11.889	1.00	117.67
20	6735	C	VAL E	79	3.081	62.669	-15.111	1.00	170.14
	6736	0	VAL E	79	4.093	62.798	-15.803	1.00	170.14
	6737 6738	N CA	TYR E TYR E	80 80	1.903 1.782	62.292	-15.605	1.00	121.68
	6739	CB	TYR E	80	1.782	62.023 60.700	-17.028 -17.272	1.00	121.68
25	6740	ĊĠ	TYR E	80	1.291	60.179	-18.675	1.00 1.00	162.42 162.42
	6741	CD1	TYR E	80	2.439	59.447	-18.995	1.00	162.42
	6742	CE1	TYR E	80	2.661	58.981	-20.301	1.00	162.42
	6743	CD2	TYR E	80	0.370	60.437	-19.696	1.00	162.42
30	6744 6745	CE2 CZ	TYR E	80	0.588	59.980	-21.002	1.00	162.42
50	6746	OH	TYR E TYR E	80 80	1.732 1.960	59.256 58.803	-21.290	1.00	162.42
	6747	C	TYR E	80	1.040	63.132	-22.557 -17.752	1.00 1.00	162.42
	6748	Ŏ	TYR E	80	0.022	63.642	-17.277	1.00	121.68 121.68
25	6749	Ņ	LEU E	81	1.562	63.511	-18.906	1.00	108.83
35	6750	CA	LEU E	81	0.943	64.545	-19.706	1.00	108.83
	6751 6752	CB CG	LEU E LEU E	81	1.930	65.677	-19.978	1.00	110.26
	6753	CD1	LEU E	81 81	1.380 0.173	66.724 67.390	-20.946	1.00	110.26
	6754	CD2	LEU E	81	2.432	67.748	-20.296 -21.292	1.00 1.00	110.26 110.26
40	6755	C	LEU E	81	0.514	63.944	-21.028	1.00	108.83
	6756	0	LEU E	81	1.308	63.312	-21.701	1.00	108.83
	6757	N	GLU E	82	-0.740	64.132	-21.407	1.00	99.21
	6758 6759	CA CB	GLU E	82	-1.194	63.601	-22.679	1.00	99.21
45	6760	CG	GLU E	82 82	-2.359 -2.479	62.625 61.592	-22.473	1.00	224.57
	6761	CD	GLU E	82	-3.618	60.615	-23.590 -23.373	1.00 1.00	224.57 224.57
	6762	OE1	GLU E	82	-3.903	60,282	-22.198	1.00	224.57 224.57
	6763	QE2	GLU E	82	-4.216	60.166	-24.380	1.00	224.57
50	6764	C	GLU E	82	-1.623	64.749	-23.596	1.00	99.21
30	6765 6766	0 N	GLU E VAL E	82 83	-2.287	65.700	-23.142	1.00	99.21
	6767	ČA	VAL E	83	-1.231 -1.599	64.670 65.690	-24.876	1.00	128.82
	6768	CB	VAL E	83	-0.388	66.250	-25.871 -26.586	1.00 1.00	128.82 97.06
	6769	CG1	VAL E	83	-0.835	67.323	-27.572	1.00	97.06
55	6770	CG2	VAL E	83	0.585	66.824	-25.562	1.00	97.06
	6771	C	VAL E	83	-2.564	65.129	-26.915	1.00	128.82
	6772 6773	O	VAL E	83	-2.424	63.998	-27.378	1.00	128.82
	6774	N CA	PHE E PHE E	84 84	-3.528 -4.572	65.951 65.524	-27.302	1.00	126.16
60	6775	CB	PHE E	84	-5.893	65.416	-28.218 -27.473	1.00 1.00	126.16 129.94
	6776	CG	PHE E	84	-5.885	64.434	-26.357	1.00	129.94
	6777	CD1	PHE E	84	-5.361	64.755	-25.107	1.00	129.94
	6778	CD2	PHE E	84	-6.432	63.191	-26.547	1.00	129.94
65	6779 6780	CE1 CE2	PHE E	84	-5.372	63.832	-24.070	1.00	129.94
05	6781	CZ	PHE E PHE E	84 84	-6.449 -5.924	62.262 62.585	·25.522	1.00	129.94
	6782	Č	PHE E	84	-3.824 -4.872	62.585 66.377	-24.278 -29.422	1.00 1.00	129.94
	6783	Ö	PHE E	84	-4.588	67.571	-29.466	1.00	126.16 126.16
70	6784	N	SER E	85	-5.510	65.732	-30.385	1.00	167.68
70	6785	CA	SER E	85	-5. 96 0	66.381	-31.604	1.00	167.68

	6786 6787	CB OG	SER E SER E	85 · 85	-5.136 -5.627	65.957 66.593	-32.815 -33.981	1.00	221.67 221.67
	6788	С	SER E	85	-7.390	65.909	-31.783	1.00	167.68
_	6789	0	SER E	85	-7.620	64.718	-32.008	1.00	167.68
5	6790	N	ASP E	86	-8.342	66.840	-31.661	1.00	124.68
	6791	CA	ASP E	86	-9.766	66.530	-31.793	1.00	124.68
	6792 6793	CB CG	ASP E ASP E	86 86	-10.199	65.550	-30.697	1.00	146.90
	6794	OD1	ASP E	86	-11.214 -12.235	64.542 64.955	-31.189 -31.792	1.00 1.00	146.90
10	6795	OD2	ASP E	86	-10.979	63.329	-30.978	1.00	146.90 146.90
	6796	C	ASP E	86	-10.583	67.792	-31.658	1.00	124.68
	6797	0	ASP E	86	-10.064	68.815	-31.244	1.00	124.68
	6798	N	TRP E	87	-11.864	67.722	-31.995	1.00	145.58
15	6799	CA CB	TRP E	87	-12.717	68.901	-31.880	1.00	145.58
13	6800 6801	CG	TRP E	87 87	-14.072 -14.077	68.644	-32.537	1.00	249.10
	6802	CD2	TRP E	87 87	-14.077	69.003 68.127	-33.989 -35.085	1.00 1.00	249.10
	6803	CE2	TRP E	87	-13.877	68.898	-36.268	1.00	249.10 249.10
	6804	CE3	TRP E	87	-13.517	J∂.759	-35.187	1.00	249.10
20	6805	CD1	TRP E	87	-14.291	70.241	-34.532	1.00	249.10
	6806	NE1	TRP E	87	-14.173	70.189	-35.899	1.00	249.10
	6807 6808	CZ2 CZ3	TRP E TRP E	87	-13.663	68.354	-37.538	1.00	249.10
•	6809	CH2	TRP E	87 87	-13.302 -13.379	66.212 67.011	-36.451	1.00	249.10
25	6810	C	TRP E	87 87	-13.379	69.314	-37.610 -30.433	1.00 1.00	249.10
	6811	ŏ	TRP E	87	-12.607	70.467	-30.077	1.00	145.58 145.58
	6812	N	LEU E	88	-13.345	68.377	-29.605	1.00	109.18
	6813	CA	LEU E	88	-13.521	68.658	-28.190	1.00	109.18
30	6814	CB	LEU E	88	-15.001	68.601	-27.819	1.00	123.07
3 0	6815 6816	CG CD1	LEU E	88	-15.885	69.659	-28.476	1.00	123.07
	6817	CD2	LEU E	88 88	-17.294 -15.326	69.581 71.049	-27.913 -28.223	1.00	123.07
	6818	C	LEU E	88	-12.715	67.699	-26.223 -27.298	1.00 1.00	123.07 109.18
	6819	ō	LEU E	88	-12.590	66.501	-27.598	1.00	109.18
35	6820	N	LEU E	89	-12.147	68.231	-26.214	1.00	123.09
	6821	CA	LEU E	89	-11.380	67.420	-25.270	1.00	123.09
	6822 6823	CB CG	LEU E	89	-9.891	67.745	-25.358	1.00	138.74
	6824	CD1	LEV E	89 89	-9.031 -9.313	66.974	-24.347	1.00	138.74
40	6825	CD2	LEU E	89	-9.515 -7.565	65.467 67.265	-24.460 -24.589	1.00 1.00	138.74
	6826	C	LEU E	89	-11.865	67.724	-23.864	1.00	138.74 123.09
	6827	0	LEU E	89	-11.959	68.879	-23.478	1.00	123.09
	6828	N	LEU E	90	-12.184	66.695	-23.097	1.00	99.50
45	6829	CA	LEU E	90	-12.659	66.912	-21.737	1.00	99.50
43	6830 6831	C8 CG	LEU E	90 90	-13.556	65.759	-21.305	1.00	113.63
	6832	CD1	LEU E	90	-13.932 -14.685	65.784 67.054	-19.817 -19.527	1.00 1.00	113.63
	6833	CD2	LEU E	90	-14.770	64.565	-19.457	1.00	113.63 113.63
	6834	С	LEU E	90	-11.502	67.023	-20.773	1.00	99.50
50	6835	0	LEU E	90	-10.779	66.046	-20.570	1.00	99.50
	6836	N	GLN E	91	-11.316	68.194	-20.170	1.00	92.89
	6837 6838	CA	GLN E	91	-10.202	68.367	-19.228	1.00	92.89
	6839	CG	GLN E	91 01	-9.505	69.690	-19.467	1.00	161.25
55	6840	CD	GLN E	91 91	-8.933 -8.254	69.836 71.177	-20.848 -21.039	1.00	161.25
	6841	OE1	GLN E	91	-8.877	72.232	-20.866	1.00 1.00	161,25 161,25
	6842	NE2	GLN E	91	-6.968	71.149	-21.398	1.00	161.25
	6843	Ç	GLN E	91	-10.632	68.289	-17.770	1.00	92.89
60	6844	0	GLN E	91	-11.680	68.833	-17.391	1.00	92.89
00	6845 6846	N CA	ALA E	92	-9.814	67.612	-16.961	1.00	113.22
	6847	CA CB	ALA E ALA E	92 92	-10.114 -10.393	67.458 65.997	-15.544 -15.212	1.00	113.22
	6848	Č	ALA E	92	-8.942	67.975	-15.212 -14.720	1.00	187.04
	6849	ō	ALA E	92	-0.34 <u>2</u> -7.777	67.802	-15.105	1.00 1.00	113.22 113.22
65	6850	N	SER E	93	-9.271	68.623	-13.596	1.00	114.34
	6851	CA	SER E	93	-8. 27 9	69.178	-12.676	1.00	114.34
	6852	CB	SER E	93	-8.973	69.762	-11.425	1.00	137.73
	6853 6854	OG C	SER E	93	-9.879	68.858	-10.813	1.00	137.73
70	6855	ŏ	SER E SER E	93 93	-7.326 -6.140	68.043 68.079	-12.300	1.00	114.34
. •		•	OCH E	3 3	-6.140	68.078	-12.593	1.00	114.34

	6856 6857 6858	N CA CB:	ALA E ALA E ALA E	94 94	-7.869 -7.113	67.028 65.858	-11.653 -11.255	1.00 1.00	121.13 121.13
	6859	C.	ALA E	94 94	-6.898 -8.008	65.855 64.684	-9.748 -11.671	1.00 1.00	206.55
5	6860	0	ALA E	94	-9.235	64.832	-11.768	1.00	121.13 121.13
	6861	N	GLU E	95	-7.424	63.520	-11.937	1.00	135.32
	6862 6863	CA CB	GLU E	95 95	-8.238 -7.496	62.378 61.564	-12.347	1.00	135.32
	6864	CG	GLU E	95	-7.262	62.342	-13.390 -14.660	1.00 1.00	189.07 189.07
10	6865	CD.	GLU E	95	-6.736	61.482	-15.780	1.00	189.07
	6866 6867	OE1 OE2	GLU E	95	-6.466	62.025	-16.876	1.00	189.07
	6868	C	GLU E	95 95	-6.596 -8.632	60.259 61.500	-15.563 -11.171	1.00 1.00	189.07
	6869	Ö	GLU E	95	-9.632	60.772	-11.247	1.00	135.32 135.32
15	6870	N	VAL E	96	-7.854	61.581	-10.085	1.00	121.52
	6871 6872	CA CB	VAL E	96 96	-8.118 -6.994	60.807	-8.865	1.00	121.52
	6873	<u>0</u> 61	VAL E	96	-0.994 -7.480	59.808 58.754	-8.591 -7.615	1.00 1.00	138.26 138.26
00	6874	CG2	VAL E	96	-6.534	59.178	-9.895	1.00	138.26
20	6875	C O·	VAL E	96	-8.237	61.741	-7.664	1.00	121.52
	6876 6877	Ň	VAL E	96 97	-7.376 -9.278	62.598 61.566	-7.462 -6.854	1.00	121.52
	6878	CA	VAL E	97	-9.458	62.462	-5.725	1.00 1.00	165.05 165.05
25	6879	CB	VAL E	97	-10.499	63.511	-6.048	1.00	119.89
23	6880 6881	CG1 CG2	VAL E	97 97	-10.338	64.666	-5.113	1.00	119.89
	6882	C	VAL E	97 97	-10.373 -9.856	63.961 61.866	-7.482 -4.380	1.00 1.00	119.89 165.05
	6883	0	VAL E	97	-10.545	60.844	-4.325	1.00	165.05
30	6884	N	MET E	98	-9.427	62.544	-3.306	1.00	159.57
50	6885 6886	CA CB	MET E	98 98	-9.713 -8.657	62.161 62.750	-1.914	1.00	159.57
	6887	ČĞ	MET E	98	-7.247	62.228	-0.973 -1.152	1.00 1.00	249.69 249.69
	6888	SD	MET E	98	-7.038	60.577	-0.463	1.00	249.69
35	6889 6890	CE C	MET E	98 98	-6.946	60.948	1.288	1.00	249.69
33	6891	ŏ	MET E	98	-11.071 -11.268	62.740 63.954	-1.522 -1.606	1.00 1.00	159.57 159.57
	6892	Ņ	GLU E	99	-11.993	61.888	-1.075	1.00	145.00
	6893	CA	GLU E	99	-13.327	62.349	-0.683	1.00	145.00
40	6894 6895	CB CG	GLU E	99 99	-13.989 -15.505	61.342 61.399	0.261 0.247	1.00	208.72
	6896	CD	GLU E	99	-16.126	60.618	1.385	1.00 1.00	208.72 208.72
	6897	OE1	GLU E	99	-15.593	59.542	1.731	1.00	208.72
	6898 6899	OE2 C	GLU E	99 99	-17.154 -13.241	61.079	1.923	1.00	208.72
45	6900	ŏ	GLU E	99	-13.241	63.699 63.854	0.022 0. 99 3	1.00 1.00	145.00 145.00
	6901	N	GLY E	100	-13.970	64.686	-0.473	1.00	140.46
	6902 6903	CA	GLY E	100	-13.941	65.989	0.164	1.00	140.46
	6904	C O	GLY E	100 100	-13.192 -13.449	67.070 68.256	-0.585	1.00	140.46
50	6905	Ň	GLN E	101	-12.279	66.679	-0.353 -1.475	1.00 1.00	140.46 158.90
	6906	CA	GLN E	101	-11.493	67.641	-2.259	1.00	158.90
	6907 6908	CB CG	GLN E	101 101	-10.255 -9.216	66.969 66. 62 5	-2.835	1.00	248.74
	6909	CD	GLN E	101	-9.216 -9.002	67.764	-1.800 1د08-1	1.00 1.00	248.74
55	6910	OE1	GLN E	101	-9.873	68.070	-0.017	1.00	248.74 248.74
	6911	NE2	GLN E	101	-7.848	68.409	-0.919	1.00	248.74
	6912 6913	C O	GLN E	101 101	-12.290 -13.445	68.324 67.007	-3.371	1.00	158.90
	6914	Ň	PRO E	102	-11.657	67.987 69.302	-3.628 -4.050	1.00 1.00	158.90 164.28
60	6915	CD	PRO E	102	-10.406	69.971	-3.720	1.00	154.28
	6916 6917	CA CB	PRO E	102	-12.358	69.987	-5.140	1.00	164.28
	6918	CG	PRO E	102 102	-11.739 -10.312	71.379 71.040	-5.074 -4.796	1.00	154.28
<i>C</i> =	6919	С	PRO E	102	-12.161	69.327	-4.796 -6.496	1.00 1.00	154.28 164.28
65	6920	0	PRO E	102	-11.119	68.720	-6.771	1.00	164.28
	6921 6922	N CA	LEV E	103 103	-13.169 -13.127	69.467	-7.358 8.670	1.00	176.34
	6923	CB	LEU E	103	-13.127	68.873 67.617	-8.679 -8.690	1.00	176.34 122.49
70	6924	CG	LEU E	103	-13.722	66.849	-9.971	1.00	122.49
70	6925	CD1	LEV E	103	-12.310	66.308	-9.883	1.00	122.49

								•	
	6926	CD2	LEU E	103	-14.724	65.736	-10.156	1.00	122.49
	6927 6928	C O :	LEU E	103	-13.618	69.805	- 9 .776	1.00	176.34
	6929	Ň	PHE E	103 104	-14.736 -12.805	70.305 70.027	-9.696	1.00	176.34
5	6930	CA	PHE E	104	-13.233	70.890	-10.806 -11.903	1.00 1.00	126.68
	6931	СВ	PHE E	104	-12.412	72.174	-11.954	1.00	126.68 239.90
	6932	CG	PHE E	104	-12.405	72.934	-10.681	1.00	239.90
	6933	CD1	PHE E	104	-11.612	72.520	-9.623	1.00	239.90
10	6934	CD2	PHE E	104	-13.201	74.060	-10.528	1.00	239.90
10	6935 6936	CE1 CE2	PHE E	104	-11.608	73.221	-8.416	1.00	239.90
	6937	CZ	PHE E PHE E	104 104	-13.211 -12.410	74.770 74.349	-9.331	1.00	239.90
	6938	Č	PHE E	104	-13.110	74.349 70.197	-8.269 -13.250	1.00 1.00	239.90
	6939	Ō	PHE E	104	-12.033	69.723	-13.600	1.00	126.68 126.68
15	6940	N	LEU E	105	-14.208	70.136	-14.003	1.00	132.08
	6941	CA	LEU E	105	-14.176	69.524	-15. 32 7	1.00	132.08
	6942 6943	CB CG	LEU E	105	-15.249	68.452	-15.456	1.00	106.14
	6944	CD1	LEU E	105 105	-15.131	67.347	-14.414	1.00	106.14
20	6945	CD2	LEU E	105	-16.174 -13.704	66.283 66.777	-14.719 -14.429	1.00	106.14
	6946	C	LEŬ E	105	-14.413	70.618	-16.344	1.00 1.00	106.14 132.08
	6947	0	LEU E	105	-15.119	71.592	-16.064	1.00	132.08
	6948	Ņ	ARG E	106	-13.848	70.456	-17.532	1.00	113.14
25	6949	CA	ARG E	106	-13.996	71.486	-18.543	1.00	113.14
23	6950 6951	CB CG	ARG E ARG E	106	-12.753	72.363	-18.492	1.00	157.66
	6952	CD	ARG E	106 106	-12.740 -11.397	73.498 74.197	-19.454	1.00	157.66
	6953	NE	ARG E	106	-11.356	75.192	-19.428 -20.478	1.00 1.00	157.66
	6954	CZ	ARG E	106	-10.256	75.566	-21.103	1.00	157.66 157.66
30	6955	NH1	ARG E	106	-9.094	75.020	-20.774	1.00	157.66
	6956	NH2	ARG E	106	-10.331	76.473	-22.071	1.00	157.66
	6957 6958	C	ARG E ARG E	106	-14.172	70.905	-19.932	1.00	113.14
	6959	N	CYS E	106 107	-13.363 -15.235	70.068 71.312	-20.365	1.00	113.14
35	6960	ĞA	CYS E	107	-15.456	70.829	-20.620 -21.979	1.00 1.00	132.92
	6961	С	CYS E	107	-14.646	71.786	-22.808	1.00	132.92 132.92
	6962	0	CYS E	107	-15.068	72.922	-22.996	1.00	132.92
	6963	СВ	CYS E	107	-16.923	70.942	-22.370	1.00	146.71
40	6964 6965	SG N	CYS E	107	-17.372	70.056	-23.927	1.00	146.71
40	6966	GA	HIS E HIS E	108 108	-13.483 -12.576	71.339 72.195	-23.282	1.00	154.76
	6967	CB	HIS E	108	-12.576	72.195 71.911	-24.052 -23.639	1.00	154.76
	6968	CG	HIS E	108	-10.136	72.910	-24.161	1.00 1.00	172.76 172.76
4.5	6969	CD2	HIS E	108	-8.957	72.738	-24.810	1.00	172.76
45	6970	ND1	HIS E	108	-10 <i>.277</i>	74.262	-23.967	1.00	172.76
	6971 6972	CE1 NE2	HIS E HIS E	108	-9.221	74.888	-24.473	1.00	172.76
	6973	C	HIS E HIS E	108 108	-8.409 -12.688	73.987 72.087	-24.986	1.00	172.76
	6974	ŏ	HIS E	108	-12.576	72.067 70.997	-25.560 -26.129	1.00	154.76
50	6975	N	GLY E	109	-12.892	73.240	-26.194	1.00 1.00	154.76 128.76
	6976	ÇA	GLY E	109	-13.007	73.287	-27.637	1.00	128.76
	6977	C	GLY E	109	-11.632	73.334	-28.260	1.00	128.76
	6978 6979	O N	GLY E	109	-10.666	73.574	-27.552	1.00	128.76
55	6980	CA	TRP E	110 110	-11.539 -10.260	73.092	-29.566	1.00	154.27
	6981	CB	TRP E	110	-10.200	73.136 72.268	-30.251 -31.503	1.00	154.27
	6982	CG	TRP E	110	-9.107	72.411	-32.397	1.00 1.00	170.55 170.55
	6983	CD2	TRP E	110	-7.963	71.539	-32.468	1.00	170.55
60	6984	CE2	TRP E	110	-7.073	72.098	-33.406	1.00	170.55
00	6985 6986	CE3	TRP E	110	-7.606	70.345	-31.825	1.00	170.55
	6987	CD1 NE1	TRP E	110 110	-8.8 63	73.422	-33.270	1.00	170.55
	6988	CZ2	TRP E	110	-7.645 -5.840	73.242 71.501	-33.877 -33.710	1.00	170.55
	6989	CZ3	TRP E	110	-6.375	69.755	-33.719 -32.137	1.00 1.00	170.55 170.55
65	6990	CH2	TRP E	110	-5.509	70.339	-33.077	1.00	170.55 170.55
	6991	C	TRP E	110	-9.897	74.586	-30.600	1.00	154.27
	6992 6993	O	TRP E	110	-10.786	75.431	-30.767	1.00	154.27
	6993 6994	N CA	ARG E ARG E	111 111	-8.5 96	74.878	-30.693	1.00	180.74
70	6995	CB	ARG E	111	-8.116 -8.361	76.229 76.580	-30. 99 4 -32.460	1.00	180.74
-				•••	-V.001	10.000	·32.40U	1.00	249.46

	6996 6997	CG CD	ARG E	111 111	-7.220 -7.366	76.198 76.870	-33.381 -34.7 3 8	1.00 1.00	249.46 249.46
•	6998 6999	NE : CZ	ARG E ARG E	111 111	-6.076	77.324	-35.248	1.00	249.46
5	7000	NH1	ARG E	111	-5.295 -5.672	78.200 78.720	-34.623 -33.463	1.00	249.46
•	7001	NH2	ARG E	111	-4.136	78.557	-35.155	1.00 1.00	249.46
	7002	С	ARG E	111	-8.804	77.263	-30.104	1.00	249.46 180.74
	7003	0	ARG E	111	-9.013	78.408	-30.490	1.00	180.74
10	7004	N	ASN E	112	-9.156	76.839	-28.903	1.00	179.60
10	7005	CA	ASN E	112	-9.815	77.702	-27.949	1.00	179.60
	7006 7007	CB CG	ASN E ASN E	112	-8.820	78.719	-27.388	1.00	235.58
	7007	OD1	ASN E	112 112	-9.314 -10.493	79.373 79.276	-26.110	1.00	235.58
	7009	ND2	ASN E	112	-8.413	80.052	-25.757 -25.412	1.00 1.00	235.58 235.58
15	7010	C	ASN E	112	-11.002	78.426	-28.579	1.00	179.60
	7011	0	ASN E	112	-11.299	79.551	-28.193	1.00	179.60
	7012	N	TRP E	113	-11.671	77.798	-29.550	1.00	181.35
	7013	CA	TRP E	113	-12.841	78.420	-30.174	1.00	181.35
20	7014 7015	CB CG	TRP E	113	-13.343	77.633	-31.368	1.00	198.74
20	7016	CD2	TRP E	113 113	-12.618 -12.345	<i>7</i> 7.902 76.965	-32.604 -33.651	1.00	198.74
	7017	CE2	TRP E	113	-11.666	77.674	-34.676	1.00 1.00	198.74 198.74
	7018	CE3	TRP E	113	-12.603	75.599	-33.823		198.74
05	7019	CD1	TRP E	113	-12.114	79.099	-33.018	1.00	198.74
25	7020	NE1	TRP E	113	-11.527	78.973	-34.267	1.00	198.74
	7021	CZ2	TRP E	113	-11.246	77.052	-35.861	1.00	198.74
	7022 7023	CZ3 CH2	TRP E	113	-12.185	74.983	-34.994	1.00	198.74
	7023	C	TRP E TRP E	113 113	-11.515 -13.968	75.711 79.479	-36.001	1.00	198.74
30	7025	ŏ	TRP E	113	-13.763	78.478 78.229	-29.164 -27.974	1.00 1.00	181.35
	7026	Ň	ASP E	114	-15.168	78.806	-29.629	1.00	181.35 198.96
	7027	CA	ASP E	114	-16.312	78.881	-28.724	1.00	198.96
	7028	CB	ASP E	114	-17.015	80.250	-28.852	1.00	241.05
35	7029	CG	ASP E	114	-16.337	81.350	-28.0 2 6	1.00	241.05
22	7030 7031	OD1 OD2	ASP E ASP E	114	-16.217	81.193	-26.790	1.00	241.05
	7032	C	ASP E	114 114	-15.928 -17.299	82.374 77.746	-28.614	1.00	241.05
	7033	ŏ	ASP E	114	-17.646	77.470 77.470	-28.994 -30.151	1.00 1.00	198.96
	7034	N	VAL E	115	-17.732	77.083	-27.922	1.00	198.96 162.46
40	7035	CA	VAL E	115	-18.686	75.985	-28.039	1.00	162.46
	7036	CB	VAL E	115	-18.191	74.726	-27.316	1.00	122.72
	7037 7038	CG1 CG2	VAL E	115	-19.018	73.528	-27.751	1.00	122.72
	7039	C	VAL E VAL E	115 115	-16.727 -20.033	74.493	-27.603	1.00	122.72
45	7040	ŏ	VAL E	115	-20.084	76.382 77.042	-27.434 -26.385	1.00	162.46
	7041	Ň	TYR E	116	-21,114	75.972	-28.096	1.00 1.00	162.46 116.01
	7042	CA	TYR E	116	-22.468	76.285	-27.648	1.00	116.01
	7043	CB	TYR E	116	-23.177	77.143	-28.693	1.00	231.08
50	7044	CG	TYR E	116	-22.540	78.498	-28.877	1.00	231.08
<i>5</i> 0	7045 7046	CD1 CE1	TYR E TYR E	116	-21.643	78.743	-29.918	1.00	231.08
	7047	CD2	TYR E TYR E	116 116	-21.024 -22.805	79.992 79.531	-30.062 -27.984	1.00	231.08
	7048	GE2	TYR E	116	-22.194	80.780	-27.984 -28.114	1.00 1.00	231.08
	7049	CZ	TYR E	116	-21.306	81.006	-29.154	1.00	231.08 231.08
55	7050	OН	TYP E	116	-20.705	82.241	-29.278	1.00	231.08
	7051	C	TYR E	116	-23.279	75.007	-27.387	1.00	116.31
	7052 7053	0	TYR E	116	-22.829	73.909	-27.722	1.00	116.01
	7053 7054	N CA	LYS E Lys e	117	-24.472	75.163	-26.792	1.00	118.22
60	7055	CB	LYS E	117 117	-25.359 -26.062	74.042 73.531	-26.454 -27.701	1.00	118.22
	7056	ČĞ	LYS E	117	-27.319	74.305	-27.701 -28.079	1.00 1.00	223.92
	7057	CD	LYS E	117	-28.221	73.481	-29.013	1.00	223.92 223.92
	7058	CE	LYS E	117	-28.639	72.150	-28.354	1.00	223.92
65	7059	NZ	LYS E	117	-29.508	71.267	-29.203	1.00	223.92
UJ	7060 7061	C	LYS E	117	-24.619	72.877	-25.764	1.00	118.22
	7061 7062	O N	LYS E	117	-24.736	71.712	-26.150	1.00	118.22
	7063	CA	VAL E VAL E	118 118	-23.883 -23.120	73.200 73.205	-24.714	1.00	129.60
	7064	CB	VAL E	118	-23.120	72.205 72.855	-23.991 -23.349	1.00 1.00	129.60
70	7065	CG1	VAL E	118	-21.403	72.044	-22.155	1.00	89.69 82 69
									00 118

	7066	CG2	VAL E	118	-20.796	72.955	-24.377	1.00	00.00
	7067	С	VAL E	118	-23.869	71.403	-22.939	1.00	89.69
	7068	0	VAL E	118	-24.702	71.913	-22.190	1.00	129.60
_	7069	N	ILE E	119	-23.522	70.124	-22.896	1.00	129.60 95.90
5	7070	CA	ILE E	119	-24.087	69.164	-21.965	1.00	95.90
	7071	CB	ILE E	119	-25.146	68.311	-22.666	1.00	119.63
	7072	CG2	ILE E	119	-25.826	67. 37 5	-21.651	1.00	119.63
	7073	CG1	ILE E	119	-26.147	69.225	-23.373	1.00	119.63
10	7074	CD1	ILE E	119	-26.848	68.560	-24.500	1.00	119.63
10	7075	C	ILE E	119	-22.989	68.219	-21.503	1.00	95.90
	7076	0	ILE E	119	-22.248	67. 66 6	-22.322	1.00	95.90
	7077	N	TYR E	120	-22.869	68.034	-20.202	1.00	107.56
	7078	CA	TYR E	120	-21.875	67.106	-19.719	1.00	107.56
15	7079	CB	TYR E	120	-21.255	67.604	-18.439	1.00	104.01
13	7080	CG	TYR E	120	-20.386	68.807	-18.628	1.00	104.01
	7081	CD1	TYR E	120	-20.926	70.082	-18.631	1.00	104.01
	7082 7083	CE1	TYR E	120	-20.114	71.219	-18.804	1.00	104.01
	7083 7084	CD2 CE2	TYR E	120	-19.015	68.678	-18.804	1.00	104.01
20	7085	CZ	TYR E	120	-18.202	69.795	-18.983	1.00	104.01
20	7086	OH	TYR E	120	-18.752	71.061	-18.983	1.00	104.01
	7087		TYR E	120	-17.939	72.151	-19.184	1.00	104.01
	7087	C	TYR E	120	-22.604	65.814	-19.436	1.00	107.56
	7089	N	TYR E	120	-23.806	65.843	-19.141	1.00	107.56
25	7090	CA	TYR E	121	-21.908	64.685	-19.536	1.00	107.48
23	7090	CB	TYR E	121	-22.543	63.401	-19.260	1.00	107.48
	7092	CG	TYR E TYR E	121	-22.756	62.594	-20.561	1.00	135.25
	7093	CD1	TYR E	121	-23.773	63.118	-21.547	1.00	135.25
	7094	CE1	TYRE	121	-23.626	64.371	-22.119	1.00	135.25
30	7095	CD2	TYR E	121 121	-24.513	64.825	-23.097	1.00	135.25
-	7096	CE2	TYR E	121	-24.837 -25.730	62.324	-21.967	1.00	135.25
	7097	cz	TYR E	121	-25.730 -25.567	62.763	-22.942	1.00	135.25
	7098	OH OH	TYR E	121	-25.567 -26.438	64.011	-23.507	1.00	135.25
	7099	Č.	TYR E	121	-21.706	64.440 62.546	-24.498	1.00	135.25
35	7100	ŏ	TYR E	121	-20.478	62.430	-18.293	1.00	107.48
	7101	Ñ	LYS E	122	-22.376	61.938	-18.440	1.00	107.48
	7102	CA	LYS E	122	-21.694	61.059	-17.315 -16.384	1.00	117.16
	7103	CB	LYS E	122	-21.760	61.615	-14.969	1.00	117.16
	7104	CG	LYS E	122	-21.046	60.734	-13.965	1.00 1.00	184.34
40	7105	CD	LYS E	122	-21.385	61.133	-12.559	1.00	184.34
	7106	CE	LYS E	122	-20.792	60.167	-11.568	1.00	184.34 184.34
	7107	NZ	LYS E	122	-21.266	60.513	-10.209	1.00	184.34
	7108	С	LYS E	122	-22.391	59.709	-16.426	1.00	117.16
45	7109	0	LYS E	122	-23.564	59.597	-16.064	1.00	117.16
45	7110	N	ASP E	123	-21.669	58.684	-16.864	1.00	145.37
	7111	CA	ASP E	123	-22.228	57.333	-16.960	1.00	145.37
	7112	CB	ASP E	123	-22.532	56.766	-15.574	1.00	150.82
	7113	CG	ASP E	123	-21 <i>.2</i> 71	56.378	-14.821	1.00	150.82
50	7114	OD1	ASP E	123	-20.424	55.649	-15.391	1.00	150.82
50	7115	OD2	ASP E	123	-21.128	56.795	-13.657	1.00	150.82
	7116	C	ASP E	123	-23.483	57.247	-17.825	1.00	145.37
	7117	0	ASP E	123	-24.508	56.696	-17.395	1.00	145.37
	7118 7119	N O4	GLY E	124	-23.389	57.796	-19.040	1.00	162.19
55	7120	CA	GLY E	124	-24.497	57.764	-19.983	1.00	162.19
<i>J J</i>	7121	C	GLY E	124	-25.683	58.666	-19.698	1.00	162.19
	7122	Ň	GLY E GLU E	124	-26.586	58.768	-20.526	1.00	162.19
	7123	ČA	GLU E	125	-25.683	59.324	-18.541	1.00	143.04
	7124	CB	GLU E	125	-26.776	60.216	-18.134	1.00	143.04
60	7125	CG	GLU E	125 125	-27.041	60.063	-16.627	1.00	249.69
	7126	CD	GLU E	125	-27.627 -29.094	58.724	-16.208	1.00	249.69
	7127	OE1	GLU E	125		58.592	-16.573	1.00	249.69
	7128	OE2	GLU E	125	-29.901 -29.440	59.390	-16.051	1.00	249.69
	7129	Č	GLU E	125	-29. 44 0 -26.510	57.696 61.600	-17.379	1.00	249.69
65	7130	ŏ	GLU E	125	-25.384	61.692	-18.437	1.00	143.04
	7131	Ň	ALA E	128	-25.364 -27.550	62.166 62.414	-18.309	1.00	143.04
	7132	CA	ALA E	126	-27.416	62.414 63.838	-18.843	1.00	144.33
	7133	CB	ALA E	126	-28.693	63.838 64.365	-19.120 -10.726	1.00	144.33
	7134	C	ALA E	126	-27.187	64.451	-19.726 -17.754	1.00	160.82
70	7135	Ō	ALA E	126	-27.835	64.054	-17.754 -16.701	1.00	144.33
			· — · -			U-1.UU-4	-16.791	1.00	144.33

	7136	N	LEU E	127	-26.285	65.419	-17.645	1.00	143.63
	7137	CA	LEU E	127	-26.002	65.998	-16.319	1.00	143.63
	7138	CB:	LEU E	127	-24.565	65.687	-15.904	1.00	101.20
5	7139 7140	CG . CD1	LEU E	127	-24.442	65.621	-14.395	1.00	101.20
	7141	CD2	LEU E	127 127	-25.446 -23.029	64.623	-13.859	1.00	101.20
	7142	Č	LEU E	127	-25.029	65.214 ∪7.484	-14.036 -16.121	1.00	101.20
	7143	Ö	LEU E	127	-27.036	67.875	-15.264	1.00 1.00	143.63
10	7144	N	LYS E	128	-25.532	68.305	-16.880	1.00	143.63 117.01
10	7145	CA	LYS E	128	-25.707	69.747	-16.812	1.00	117.01
	7146 7147	CB CG	LYS E	128	-24.508	70.394	-16.141	1.00	217.61
	7148	CD	LYS E Lys e	128 128	-24.263 -25.300	69.930 70.474	-14.718	1.00	217.61
	7149	CE	LYS E	128	-24.958	70.474	-13 748 -12.316	1.00 1.00	217.61
15	7150	NZ	LYS E	128	-25.780	70.793	-11 306	1.00	217.61 217.61
	7151	C	LYS E	128	-25.842	70.272	-18.245	1.00	117.01
	7152 7153	0	LYS E	128	-25.417	69.599	-19.194	1.00	117.01
	7153	N CA	TYR E TYR E	129 129	-26.424	71.461	-18.406	1.00	145.51
20	7155	CB	TYR E	129	-26.601 -27.928	2.029 71.565	-19.736 -20.322	1.00	145.51
	7156	CG	TYR E	129	-28.368	72.425	-21.479	1.00 1.00	135.80 135.80
	7157	CD1	TYR E	129	-27.913	72.180	-22.768	1.00	135.80
	7158	CE1	TYR E	129	-28.292	73.003	-23.829	1.00	135.80
25	7159 7160	CD2 CE2	TYR E TYR E	129	-29.214	73.521	-21.273	1.00	135.80
	7161	CZ	TYR E	129 129	-29.599 -29.135	74.344 74.078	-22.318	1.00	135.80
	7162	OH	TYR E.	129	-29.523	74.878	-23.595 -24.643	1.00 1.00	135.80 135.80
	7163	Ç	TYR E	129	-26.557	73.557	-19.774	1.00	145.51
30	7164	0	TYR E	129	-27.124	74.221	-18.907	1.00	145.51
30	7165 7166	N CA	TRP E	130	-25.900	74.105	-20.800	1.00	157.70
	7167	CB	TRP E	130 130	-25.786 -24.539	75.554 76.108	-20.976 -20.279	1.00	157.70
	7168	CG	TRP E	130	-24.287	75.631	-18.878	1.00 1.00	223.39 223.39
35	7169	CD2	TRP E	130	-24.485	76.370	-17.677	1.00	223.39
33	7170 7171	CE2 CE3	TRP E	130	-24.066	75.557	-16.598	1.00	223.39
	7172	CD1	TRP E TRP E	130 130	-24.971 -23.782	77.660 74.419	-17.393	1.00	223.39
	7173	NE1	TRP E	130	-23.638	74.364	-18.498 -17.134	1.00 1.00	223.39 223.39
40	7174	CZ2	TRP E	130	-24.117	75.974	-15.268	1.00	223.39
40	7175	CZ3	TRP E	130	-25.023	78.083	-16.063	1.00	223.39
	7176 7177	CH2 C	TRP E TRP E	130 130	-24.605	77.238	-15.018	1.00	223.39
	7178	ŏ	TRP E	130	-25.699 -25.526	75.944 75.103	-22.451 -23.321	1.00 1.00	157.70
	7179	N	TYR E	131	-25.812	77.239	-22.718	1.00	157.70 154.17
45	7180	CA	TYR E	131	-25.721	77.775	-24.074	1.00	154.17
	7181 7182	CB CG	TYR E	131	-26.551	79.040	-24.193	1.00	200.28
	7183	CD1	TYR E TYR E	131 131	-26.730 -27.576	79.484	-25.605	1.00	200.28
	7184	CE1	TYR E	131	-27.722	78.794 79.186	-26.465 -27.789	1.00 1.00	200.28
50	7185	CD2	TYR E	131	-26.028	80.579	-26.100	1.00	200.28 200.2£
	7186	CE2	TYR E	131	-26.166	80.979	-27.426	1.00	200.28
	7187 7188	CZ OH	TYR E TYR E	131	-27.012	80.277	-28.267	1.00	200.28
	7189	C	TYR E	131 131	-27.129 -24.238	80.671 78.105	-29.584	1.00	200.28
55	7190	Ō	TYR E	131	-23.462	77.259	-24.250 -24.690	1.00 1.00	154.17 154.1,
	7191	N	GLU E	132	-23.848	79.340	-23.930	1.00	210.53
	7192	CA	GLU E	132	-22.436	79.713	-23.979	1.00	210.53
	7193 7194	CB CG	GLU E	132	-22.234	81.158	-23.507	1.00	249.69
60	7195	CD	GLU E	132 132	-22.565 -21.342	82.244 83.062	-24.531 -24.912	1.00	249.69
	7196	OE1	GLU E	132	-20.307	82.939	-24.219	1.00 1.00	249.69 249.69
	7197	OE2	GLU E	132	-21.411	83.832	-25.895	1.00	249.69
	7198	C	GLU E	132	-21.980	78.737	-22.905	1.00	210.53
65	7199 7200	O N	GLU E ASN E	132	-22.554	78.723	-21.809	1.00	210.53
	7201	CA	ASN E	133 133	-20.962 -20.610	77.929 76.931	-23.182 -22.193	1.00	143.28
	7202	СВ	ASN E	133	-19.691	75.833	-22.193 -22.820	1.00 1.00	143.28 158.57
	7203	CG	ASN E	133	-18.215	76.179	-22.850	1.00	158.57
70	7204 7205	OD1 ND2	ASN E	133	-17.820	77.296	-23.201	1.00	158.57
	, =00	NUZ	ASN E	133	-17.378	75.183	-22.520	1.00	158.57

		_							
	7206	Ç	ASN E	133	-20.152	77.365	-20.796	1.00	143.28
	7207	0	ASN E	133	-20.202	78.541	-20.431	1.00	143.28
	7208	N	HIS E	134	-19.772	76.381	-19. 99 5	1.00	154.96
5	7209	CA	HIS E	134	-19.363	76.622	-18.635	1.00	154.96
J	7210	CB	HIS E	134	-20.574	76.432	-17.724	1.00	249.69
	7211	CG	HIS E	134	-20.319	76.834	-16.296	1.00	249.69
	7212	CD2	HIS E	134	-20.339	76.096	-15.160	1.00	249.69
	7213	ND1	HIS E	134	-19.981	78.107	-15.945	1.00	249.69
10	7214	CE1	HIS E	134	-19.792	78.160	-14.625	1.00	249.69
10	7215	NE2	HIS E	134	-20.003	76.958	-14.134	1.00	249.69
	7216	C	HIS E	134	-18.282	75.617	-18.297	1.00	154.96
	7217	0	HIS E	134	-17.703	74.988	-19.184	1.00	154.96
	7218	N	ASN E	135	-18.018	75.457	-17.009	1.00	128.43
15	7219 7220	CA	ASN E	135	-17.003	74.531	-16.537	1.00	128.43
15	7221	CB CG	ASN E	135	-15.677	75.279	-16.366	1.00	226.02
	7222	OD1	ASN E ASN E	135	-15.086	75.721	-17.696	1.00	226.02
	7223	ND2	ASN E	135	-15.047	74.928	-18.643	1.00	226.02
	7224	C	ASN E	135 135	-14.602	76.963	-17.776	1.00	226.02
20	7225	ŏ	ASN E	135	-17.436 -17.046	73.896	-15.226	1.00	128.43
-0	7226	Ň	ILE E	136	-17.046	74.363	-14.166	1.00	128.43
	7227	CA	ILE E	136	-18.788	72.842 72.102	-15.318	1.00	149.25
	7228	CB	ILE E	136	-19.268	72.102	-14.159	1.00	149.25
	7229	CG2	ILE E	136	-18.140	69. 9 55	-14.588	1.00	170.48
25	7230	CG1	ILE E	136	-19.748	69.897	-15.266 -13.378	1.00	170.48
	7231	CD1	ILE E	136	-20.169	68.485	-	1.00	170.48
	7232	Č	ILE E	136	-17.824	71.949	-13. 72 6 -12. 97 5	1.00	170.48
	7233	ŏ	ILE E	136	-16.894	71.133	-13.008	1.00	149.25
	7234	Ň	SER E	137	-18.096	72.718	-11.918	1.00 1.00	149.25
30	7235	CA	SER E	137	-17.258	72.738	-10.724	1.00	150.66
	7236	СВ	SER E	137	-16.914	74.185	-10.367	1.00	150.66
	7237	OG	SER E	137	-16.282	74.247	-9.104	1.00	213.03 213.03
	7238	С	SER E	137	-17.783	72.047	-9.478	1.00	150.66
~-	7239	0	SER E	137	-18.969	72.041	-9.203	1.00	150.66
35	7240	N	ILE E	138	-16.853	71.504	-8.709	1.00	157.82
	7241	CA	ILE E	138	-17.154	70.795	-7.483	1.00	157.82
	7242	CB	ILE E	138	-17.060	69.286	-7.712	1.00	122.12
	7243	CG2	ILE E	138	-17.033	68.548	-6.388	1.00	122.12
40	7244	CG1	ILE E	138	-18.240	68.834	-8.550	1.00	122.12
40	7245	CD1	ILE E	138	-18.110	67.429	-9.027	1.00	122.12
	7246	Ç	ILE E	138	-16.219	71.180	-6.339	1.00	157.82
	7247	0	ILE E	138	-15.000	71.039	-6.435	1.00	157.82
	7248	N	THR E	139	-16.813	71.655	-5.251	1.00	216.52
45	7249 7250	CA CB	THR E	139	-16.073	72.066	-4.067	1.00	216.52
73	7250 7251	OG1	THR E	139	-16.922	73.033	-3.250	1.00	203.55
	7252	CG2	THR E	139 139	-18.202	72.437	-2.992	1.00	203.55
	7253	C	THR E	139	-17.135	74.324	-4.026	1.00	203.55
	7254	ŏ	THR E	139	-15.745 -14.637	70.839	-3.224	1.00	216.52
50	7255	Ň	ASN E	140	-14.637 -16.726	70.307 70.402	-3.273	1.00	216.52
	7256	ČA	ASN E	140	-16.589	69.224	-2.446	1.00	176.56
	7257	CB	ASN E	140	-17.543	69.336	-1.603 -0.405	1.00	176.56
	7258	CG	ASN E	140	-17.486			1.00	249.69
	7259	OD1	ASN E	140	-17.585	68.128 66.992	0. 504 0. 040	1.00	249.69
55	7260	ND2	ASN E	140	-17.347	68.365	1.805	1.00 1.00	249.69
	7261	С	ASI. E	140	-16.974	68.036	-2.490	1.00	249.69 176.56
	7262	0	ASN E	140	-18.084	67.989	-3.026	1.00	176.56
	7263	N	ALA E	141	-16.060	67.084	-2.648	1.00	151.69
	7264	CA	ALA E	141	-16.311	65.924	-3.498	1.00	151.69
60	7265	CB	ALA E	141	-15.045	65.594	-4.302	1.00	113.23
	7266	С	ALA E	141	-16.816	64.665	-2.788	1.00	151.69
	7267	0	ALA E	141	-16.218	64.183	-1.826	1.00	151.69
	7268	N	THR E	142	-17.925	64.133	-3.292	1.00	151.96
~=	7269	CA	THR E	142	-18.534	62.921	-2.754	1.00	151.96
65	7270	CB	THR E	142	-20.050	62.908	-2.974	1.00	230.06
	7271	OG1	THR E	142	-20.612	64.142	-2.510	1.00	230.06
	7272	CG2	THR E	142	-20.678	61.760	-2.218	1.00	230.06
	7273	C	THR E	142	-17.947	61.753	-3.520	1.00	151.96
70	7274	0	THR E	142	-17.415	61.923	-4.625	1.00	151.96
70	7275	N .	VAL E	143	-18.040	60.560	-2.949	1.00	131.28

	7276 7277 7278	CA CB CG1	VAL E VAL E VAL E	143 143 143	-17.493 -17.368 -18.738	59.381 58.167 57.589	-3.631 -2.692 -2.393	1.00	131.28 141.04
5	7279 7280 7281	C C CG5.	VAL E VAL E VAL E	143 143	-16.485 -18.402	57.127 58.987	-3. 32 2 -4.781	1.00 1.00 1.00	141.04 141.04 131.28
	7282 7283	N CA	GLU E GLU E	143 144 144	-17.971 -19.667 -20.614	58.336 59.388 59.063	-5.719 -4.697 -5.746	1.00 1.00 1.00	131.28 177.47 177.47
10	7284 7285 7286	CB CG CD	GLU E GLU E GLU E	144 144 144	-22.048 -22.470 -22.694	59.323 58.500 59.353	-5.298 -4.105 -2.886	1.00 1.00 1.00	249.69 249.69
	7287 7288 7289	OE1 OE2 C	GLU E GLU E GLU E	144 144 144	-23.589 -21.977 -20.316	60.221 59.167 59.875	-2.939 -1.880 -6.986	1.00 1.00	249.69 249.69 249.69
15	7290 7291 7292	O N CA	GLU E ASP E ASP E	144 145 145	-20.847 -19.467	59.583 60.895	-8.050 -6.851	1.00 1.00 1.00	177.47 177.47 122.39
20	7293 7294 7295	CB CG	ASP E ASP E	145 145	-19.091 -18.410 -19.396	61.723 62.997 64.013	-7.994 -7.532 -7.012	1.00 1.00 1.00	122.39 174.03 174.03
20	7296 7297	OD1 OD2 C	ASP E ASP E ASP E	145 145 145	-20.326 -19.244 -18.165	64.372 64.459 60.969	-7.768 -5.854 -8.943	1.00 1.00 1.00	174.03 174.03 122.39
25	7298 7299 7300	O N CA	ASP E SER E SER E	145 146 146	-17.996 -17.580 -16.672	61.363 59.870 59.031	-10.098 -8.458 -9.263	1.00 1.00 1.00	122.39 134.53 134.53
	7301 7302 7303	CB C	SER E SER E SER E	146 146 146	-16.037 -15.340 -17.412	57.940 58.481 58.362	-8.393 -7.281 -10.418	1.00 1.00 1.00	131.44 131.44 134.53
30	7304 7305 7306	O N CA	SER E GLY E GLY E	146 147 147	-18.431 -16.892 -17.542	57.729 58.500 57.888	-10.211 -11.628 -12.769	1.00 1.00 1.00	134.53 156.93
	7307 7308 7309	C O N	GLY E GLY E THR E	147 147 148	-16.839 -15.656 -17.559	58.176 58.545 58.006	-14.083 -14.095	1.00 1.00	156.93 156.93 156.93
35	7310 7311 7312	CA CB OG1	THR E THR E THR E	148 148 148	-16.993 -16.985	58.263 56.964	-15.194 -16.530 -17.380	1.00 1.00 1.00	115.73 115.73 136.83
40	7313 7314 7315	CG2 C	THR E	148 148	-18.127 -17.031 -17.755	56.934 55.746 59.409	-18.238 -16.476 -17.266	1.00 1.00 1.00	136.83 136.83 115.73
40	7316 7317	N CA	THR E TYR E TYR E	148 149 149	-18.927 -17.068 -17.660	59.283 60.533 61.699	-17.642 -17.457 -18.084	1.00 1.00 1.00	115.73 98.03 98.03
45	7318 7319 7320	CB CG CD1	TYR E TYR E TYR E	149 149 149	-17.292 -17.670 -16.951	62.968 62.986 62.244	-17.301 -15.828 -14.885	1.00 1.00 1.00	106.49 106.49 106.49
	7321 7322 7323	CE1 CD2 CE2	TYR E TYR E TYR E	149 149 149	-17.293 -18.740 -19.081	62.279 63.766 63.812	-13.545 -15.378 -14.046	1.00 1.00 1.00	106.49 106.49 106.49
50	7324 7325 7326	CZ OH C	TYR E TYR E TYR E	149 149 149	-18.358 -18.715 -17.229	63.065 63.098 61.914	-13.137 -11.815 -19.518	1.00 1.00 1.00	106.49 106.49 98.03
	7327 7328 7325	O N CA	TYR E TYR E TYR E	149 150 150	-16.224 -18.002 -17.780	61.346 62.767 63.194	-19.972 -20.200 -21.595	1.00 1.00 1.00	98.03 87.55
55	7336 7331 7332	CB CG CD1	TYR E TYR E TYR E	150 150 150	-18.019 -19.456 -20.224	62.028 61.684 62.527	-22.591 -22.936 -23.739	1.00 1.00	87.55 125.01 125.81
60	7333 7334 7335	CE1 CD2 CE2	TYR E TYR E TYR E	150 150 150	-21.551 -20.041 -21.371	62.200 60.496	-24.087 -22.482	1.00 1.00 1.00	125.81 125.81 125.81
	7336 7337 7338	CZ OH C	TYR E TYR E	150 150	-22.116 -23.405	60.157 61.018 60.699	-22.828 -23.631 -23.991	1.00 1.00 1.00	125.81 125.81 125.81
65	7339 7340 7341	O N	TYR E TYR E CYS E	150 150 151	-18.765 -19.801 -18.456	64.338 64.418 65.235	-21.835 -21.160 -22.763	1.00 1.00 1.00	87.55 87.55 108.53
	7342 7343	CA C O	CYS E CYS E	151 151 151	-19.370 -19.724 -19.030	66.343 66.457 65.919	-23.043 -24.522 -25.385	1.00 1.00 1.00	108.53 108.53 108.53
70	7344 7345	CB SG	CYS E	151 151	-18.749 -17.166	67.647 68.090	-22.588 -23.414	1.00 1.00	127.42 127.42

	7346	N	THR E	100	00.016	~ 454			
	7347	ČA	THR E	152 152	-20.816 -21.249	67.151 67.242	-24.810	1.00	109.73
	7348	CB:	THR E	152	-21.248 -22.546	67.343 66.577	-26.184	1.00	109.73
`	7349	OG1	THR E	152	-22.546	67.242	-26.478	1.00	160.87
5	7350	CG2	THR E	152	-22.443	65.158	-25.840 -25.963	1.00	160.87
	7351	C	THR E	152	-21.530	68.832	-26.420	1.00 1.00	160.87
	7352	Ó	THR E	152	-21.983	69.541	-25.509	1.00	109.73
	7353	N	GLY E	153	-21.284	69.305	·27.640	1.00	109.73
	7354	CA	GLY E	153	-21.530	70.706	-27.927	1.00	146.21 146.21
10	7355	С	GLY E	153	-21.486	71.046	-29.398	1.00	146.21
	7356	0	GLY E	153	-21.040	70.244	-30.204	1.00	146.21
	7357	N	LYS E	154	-21.947	72.247	-29.739	1.00	118.16
	7358	CA	LYS E	154	-21.973	72.704	-31.114	1.00	118.16
1.5	7359	CB	LYS E	154	-23.332	73.316	-31.423	1.00	235.84
15	7360	CG	LYS E	154	-23.517	73.732	-32.861	1.00	235.84
	7361	CD	LYS E	154	-24.925	74.260	-33.087	1.00	235.84
	7362	CE	LYS E	154	-25.120	74.744	-34.517	1.00	235.84
	7363 7364	NZ	LYS E	154	-26.493	75.280	-34.746	1.00	235.84
20	7365	C	LYS E	154	-20.864	73.716	-31.376	1.00	118.16
20	7366	0 N	LYS E Val e	154	-20.821	74.780	-30.758	1.00	118.16
	7367	CA	VAL E VAL E	155	-19.957	73.364	-32.288	1.00	164.34
	7368	CB	VAL E	155 155	-18.825	74.214	-32.686	1.00	164.34
	7369	CG1	VAL E	155	-17.520 -16.369	73.384 74.233	-32.768	1.00	138.01
25	7370	CG2	VAL E	155	-17.198	72.808	-33.254	1.00	138.01
	7371	C	VAL E	155	-19.166	72.606 74.746	-31.398	1.00	138.01
	7372	ŏ	VAL E	155	-19.503	73.962	-34.073 -34.965	1.00	164.34
	7373	Ň	TRP E	156	-19.058	76.060	-34.268	1.00	164.34
	7374	CA	TRP E	156	-19.413	76. 66 5	-35.557	1.00 1.00	249.37
30	7375	CB	TRP E	156	-18.639	76.057	-36.746	1.00	249.37 249.69
	7376	CG	TRP E	156	-17.160	76.335	-36.808	1.00	249.69
	7377	CD2	TRP E	156	-16.521	77.599	-37.045	1.00	249.69
	7378	CE2	TRP E	156	-15.126	77.369	-37.030	1.00	249.69
25	7379	CE3	TRP E	156	-16.992	78.898	-37.283	1.00	249.69
35	7380	CD1	TRP E	156	-16.152	75.425	-36.653	1.00	249.69
	7381	NE1	TRP E	156	-14.929	76.035	-36.786	1.00	249.69
	7382	CZ2	TRP E	156	-14.197	78.389	-37.233	1.00	249.69
	7383	CZ3	TRP E	156	-16.067	79.915	-37.486	1.00	249.69
40	7384 7385	CH2	TRP E	156	-14.684	79.652	-37.459	1.00	249.69
₩	7386	C O	TRP E	156	-20.881	76.332	-35.750	1.00	249.37
	7387	N	TRP E GLN E	156	-21.762	77.001	-35.194	1.00	249.37
	7388	CA	GLN E	157	-21.128	75.279	-36.536	1.00	132.72
	7389	CB	GLN E	157 157	-22.489	74.837	-36.802	1.00	132.72
45	7390	CG	GLN E	157	-23.006 -23.387	75.460 76.941	-38.103	1.00	249.69
	7391	CD	GLN E	157	-23.567 -24.572	76.941 77.181	-37.974 -37.037	1.00	249.69
	7392	OE1	GLN E	157	-25.685	76.713	-37.037 -37. 29 1	1.00	249.69
	7393	NE2	GLN E	157	-24.334	77.914	-35.949	1.00 1.00	249.69
	7394	C	GLN E	157	-22.668	73.317	-36.834	1.00	249.69
50	7395	0	GLN E	157	-23.628	72.812	-37.423	1.00	132.72 132.72
	7396	N	LEU E	158	-21.756	72.587	-36.195	1.00	229.55
	7397	CA	LEV E	158	-21.863	71.130	-36.137	1.00	229.55
	7398	CB	LEU E	158	-20.818	70.467	-37.038	1.00	228.12
	7399	CG	LEU E	158	-21.063	70.461	-38.553	1.00	228.12
55	7400	CD1	LEU E	158	-20.552	69.140	-39.108	1.00	228.12
	7401	CD2	LEU E	158	-22.544	70.590	-38.874	1.00	238.12
	7402	C	LEU E	158	-21.716	70.605	-34.713	1.00	229.55
	7403	0	LEU E	158	-21.041	71.216	-33.885	1.00	229.55
60	7404	N	ASP E	159	-22.357	69.472	-34.438	1.00	199.14
oo	7405 7406	CA	ASP E	159	-22.299	68.862	-33.114	1.00	199.14
	7400	CB CG	ASP E	159	-23.567	68.050	-32.848	1.00	198.75
	7408	OD1	ASP E ASP E	159	-24.829	68.854	-33.075	1.00	198.75
	7409	OD2		159	-25.033	69.866	-32.365	1.00	198.75
65	7410	C	ASP E ASP E	159 150	-25.613	68.475	-33.970	1.00	198.75
	7411	ŏ	ASP E	159 150	-21.082 -20.656	67.948	-32.988	1.00	199.14
	7412	N	TYR E	159 160	-20.656 -20.522	67.333 67.967	-33.963	1.00	199.14
	7413	CA CA	TYR E	160	-20.522 -19.368	67.867 67.017	-31.784	1.00	164.98
	7414	CB	TYR E	160	-18.071	67.017 67.782	-31.543 -31.730	1.00	164.98
70	7415	ČĞ	TYR E	160	-17.959	67.762 68.445	-31.730 -33.079	1.00	170.02
					500	····	-50.073	1.00	170.02

	7416 7417	CD1 CE1	TYR E	160 -18.42		-33.285	1.00	170.02
	7417 7418	CD2	TYR E TYR E	160 -18.29 160 -17.36		-34.516	1.00	170.02
	7419	CE3.	TYR E	160 -17.36; 160 -17.22;		-34.147 -35.390	1.00	170.02
5	7420	CZ	TYR E	160 -17.68		-35.562	1.00 1.00	170.02
	7421	ОН	TYR E	160 -17.51		-36.771	1.00	170.02 170.02
	7422	С	TYR E	160 -19.389		-30.153	1.00	164.98
	7423	0	TYR E	160 -19.84		-29.185	1.00	164.98
10	7424	N	GLU E	161 -18.86		-30.073	1.00	121.76
10	7425	CA CB	GLU E	161 -18.80		-28.835	1.00	121.76
	7426 7427	CG	GLU E	161 -19.43		-29.104	1.00	238.30
	7428	CD	GLU E	161 -19.437 161 -20.385		-27.962	1.00	238.30
	7429	OE1	GLU E	161 -20.217		-28.227 -27.596	1.00 1.00	238.30
15	7430	OE2	GLU E	161 -21.310		-29.058	1.00	238.30 238.30
	7431	С	GLU E	161 -17.340		-28.425	1.00	121.76
	7432	0	GLU E	161 -16.464		-29.275	1.00	121.76
	7433	N	SER E	162 -17.079		-27.125	1.00	141.30
20	7434	CA	SER E	162 -15.712		-26.603	1.00	141.30
20	7435 7436	CB OG	SER E SER E	162 -15.579		-25.350	1.00	137.77
	7437	c	SER E	162 -16.423 162 -15.318		-24.305	1.00	137.77
	7438	ŏ	SER E	162 -16.181		-26.240 -26.067	1.00 1.00	141.30
	7439	N	GLU E	163 -14.015		-26.132	1.00	141.30 137.45
25	7440	CA	GLU E	163 -13,553		-25.739	1.00	137.45
	7441	CB	GLU E	163 -12.021	61.264	-25.770	1.00	249.69
	7442	CG	GLU E	163 -11.400		-27.169	1.00	249.69
	7443 7444	CD	GLU E	163 -11.585		-27.826	1.00	249.69
30	7444 7445	OE1 OE2	GLU E GLU E	163 -11.171 163 -12.138		-27.226	1.00	249.69
50	7446	C	GLU E	163 -14.057		-28.944 -24.309	1.00	249.69
	7447	ŏ	GLU E	163 -14.182		-23.593	1.00 1.00	137.45 137.45
	74 4 8	N	PRO E	164 -14.377		-23.877	1.00	95.03
25	7449	CD	PRO E	164 -14.382		-24.662	1.00	218.77
35	7450	CA	PRO E	164 -14.877		-22.521	1.00	95.03
	7451 7452	CB	PRO E	164 -15.570		-22.657	1.00	218.77
	7452 7453	CG C	PRO E PRO E	164 -14.657 164 -13.761		-23.594	1.00	218.77
	7454	ŏ	PRO E	164 -13.761 164 -12.660		-21.475 -21.764	1.00 1.00	95.03
40	7455	Ň	LEU E	165 -14.046		-20.267	1.00	95.03 132.61
	7456	CA	LEU E	165 -13.021		-19.240	1.00	132.61
	7457	CB	LEU E	165 -12.581		-19.014	1.00	87.30
	7458	CG	LEU E	165 -11.475		-17.979	1.00	87.30
45	7459 7460	CD1 CD2	LEU E	165 -10.446		-18.043	1.00	87.30
73	7461	C	LEU E	165 -10.812 165 -13.411		-18.220	1.00	87.30
	7462	ŏ	LEU E	165 -14.470		-17.905 -17.367	1.00 1.00	132.61
	7463	Ň	ASN E	166 -12.545		-17.364	1.00	132.61 112.66
~~	7464	CA	ASN E	16U -12.794		-16.068	1.00	112.66
50	7465	CB	ASN E	166 -12.116	56.693	-16.002	1.00	172.55
	7466	CG	ASN E	166 -13.038		-16.402	1.00	172.55
	7467	OD1	ASN E	166 -14.264		-16.328	1.00	172.55
	7468 7469	ND2 C	ASN E ASN E	166 -12.445		-16.804	1.00	172.55
55	7470	ŏ	ASN E	166 -12.294 166 -11.246		-14.909	1.00	112.66
	7471	Ň	II.E E	167 -13.032		-14.999 -13.807	1.00 1.00	112.66 147.51
	7472	CA	ILE E	167 -12.643		-12.628	1.00	147.51
	7473	CB	ILE E	167 -13.409		-12.546	1.00	109.60
۲۸	7474	CG2	ILE E	167 -13.051	61.688	-11.260	1.00	109.60
60	7475	CG1	ILE E	167 -13.086		-13.760	1.00	109.60
	7476 7477	CD1 C	ILE E	167 -13.847		-13.806	1.00	109.60
	7478	ŏ	ILE E	167 -12.904 167 -14.007		-11.343	1.00	147.51
	7479	Ň	THR E	168 -11.903		-11.115 -10.481	1.00	147.51
65	7480	ČA	THR E	168 -12.093		-10.481 -9.251	1.00 1.00	104.75 104.75
	7481	CB	THR E	168 -11.250		-9.263	1.00	148.63
	7482	OG1	THR E	168 -11.607		-10.408	1.00	148.63
	7483	CG2	THR E	168 -11.516		-8.014	1.00	148.63
70	7484 7485	C	THR E	168 -11.831	58.886	-7.956	1.00	104.75
, 0	7400	0	THR E	168 -10.763	59.432	-7.718	1.00	104.75

	7400	•							
	7486 7487	N CA	VAL E VAL E	169 169	-12.849	58.924	-7.117	1.00	128.03
	7488	CB.	VAL E	169	-12.771 -14.028	59.592 60.478	-5. 83 5 -5.592	1.00	128.03
_	7489	CG1	VAL E	169	-14.231	60.741	-4.125	1.00 1.00	104.73 104.73
5	7490	CG2	VAL E	169	-13.853	61.798	-6.296	1.00	104.73
	7491	C	VAL E	169	-12.683	58.492	-4.783	1.00	128.03
	7492 7493	Ň	VAL E	169 170	-13.645 -11.510	57.767 59.262	-4.542 4.171	1.00	128.03
	7494	ČA	ILE E	170	-11.265	58.363 57.356	-4.171 -3.135	1.00 1.00	164.43
10	7495	СВ	ILE E	170	-9.826	56.804	-3.258	1.00	164.43 148.98
	7496	CG2	ILE E	170	-9.566	56.357	-4.685	1.00	148.98
	7497 7498	CG1 CD1	ILE E	170	-8.816	57.897	-2.906	1.00	148.98
	7498 7499	CD-I	ILE E ILE E	170 170	-7.368 -11.467	57.440 57.069	-2.961	1.00	148.98
15	7500	ŏ	ILE E	170	-11.524	57.968 59.184	-1.744 -1.610	1.00 1.00	164.43
	7501	N	LYS E	171	-11.560	57.141	-0.709	1.00	164.43 181.58
	7502	CA	LYS E	171	-11.775	57.672	0.633	1.00	181.58
	7503 7504	CB CG	LYS E LYS E	171	-13.118	57.176	1.157	1.00	249.69
20	750 5	CD	LYS E	171 171	-13.230 -14.675	55.666 55.211	1.123 0.996	1.00	249.69
	7506	CE	LYS E	171	-15.530	55.712	2.154	1.00 1.00	249.69 249.69
	7 507	NZ	LYS E	171	-16.931	55.206	2.058	1.00	249.69
	7508	C	LYS E	171	-10.673	57.327	1.632	1.00	181.58
25	7509 7510	O C1	LYS E	171 221	-10.810 2.209	57.585 70.540	2.833	1.00.	181.58
	7511	C2	NAG E	221	0.889	79.546 80.273	-26.386 -26.643	1.00 1.00	249.69
	7512	N2	NAG E	221	-0.170	79.298	-26.828	1.00	249.69 249.69
	7513	C 7	NAG E	221	-1.431	79.634	-26.596	1.00	249.69
30	7514 7515	O7	NAG E	221	-1.768	80.762	-26. 23 5	1.00	249.69
30	7515 7516	C8 · C3	NAG E NAG E	221 221	-2.476 1.001	78.553	-26.806	1.00	249.69
	7517	os os	NAG E	221	-0.178	81.165 81.953	-27.881 -28.009	1.00 1.00	249.69
	7518	C4	NAG E	221	2.237	82.087	-27.816	1.00	249.69 249.69
35	7519	04	NAG E	221	2.396	82.690	-29.116	1.00	249.69
33	7520 7521	C5 O5	NAG E NAG E	221	3.502	81.275	-27.447	1.00	249.69
	7521 7522	C6	NAG E	221 221	3.276 4.726	80.502 82.136	-26.244 -27.185	1.00 1.00	249.69
	7523	O 6	NAG E	221	4.477	83.098	-27.165 -26.171	1.00	249.69 249.69
40	7524	C1	NAG E	222	3.181	83.831	-29.256	1.00	249.69
40	7525 7526	C2	NAG E	222	2.456	84.839	-30.180	1.00	249.69
	7527	N2 C7	NAG E NAG E	222 222	1.186 0.936	85.239 86.518	-29.587	1.00	249.69
	7528	O7	NAG E	222	1.741	87.429	-29.301 -29.516	1.00 1.00	249.69 249.69
4 ~	7529	C8	NAG E	222	-0.420	86.835	-28.681	1.00	249.69 249.69
45	7530	C3	NAG E	222	2.220	84.191	-31.568	1.00	249.69
	7531 7532	O3 C4	NAG E NAG E	222 222	1.662	85.147	-32.469	1.00	249.69
	7533		NAG E	222	3.543 3.281	83.638 82.909	-32.143 -33.338	1.00 1.00	249.69
	7534	C5	NAG E	222	4.233	82.718	-31.115	1.00	249.69 249.69
50	7535	O5	NAG E	222	4.427	83.426	-29.859	1.00	249.69
	7536 7537	C6 O6	NAG E	222	5.592	82.211	-31.572	1.00	249.69
	7537 7538	00 C1	NAG E NAG E	222 242	5.701 7.147	80.806 50.017	-31.409	1.00	249.69
	7539	C2	NAG E	242	7.463	59.017 59.646	-23.850 -25.212	1.00 1.00	193.96
55	7540	N2	NAG E	242	8.286	60.830	-25.064	1.00	193.96 193.96
	7541	C7	NAG E	242	9.478	60.868	-25.645	1.00	1ຍປ.96
	7542 7543	O7 C8	NAG E	242	9.927	59.930	-26.305	1.00	193.96
	7544	C3	NAG E NAG E	242 242	10.299 6.151	62.130 59.995	-25.465 -25.913	1.00	193.96
60	7545	O 3	NAG E	242	6.418	60.545	-25.913 -27.194	1.00 1.00	193.96 193.96
	7546	C4	NAG E	242	5.284	58.740	-26.060	1.00	193.96
	7547 7540	04 05	NAG E	242	3.983	59.116	-26.5 6 6	1.00	193.96
	7548 7549	C5 O5	NAG E	242	5.124	58.005	-24.698	1.00	193.96
65	7549 7550	C6	NAG E NAG E	242 242	6.411 4.509	57.799 56.624	-24.050 -24.872	1.00	193.96
	7551	06	NAG E	242	3.211	56.624 56.550	-24.872 -24.304	1.00 1.00	193.96 193.96
	7552	C1	NAG E	243	3.598	58.568	-27.770	1.00	215.12
	7553	C2	NAG E	243	2.085	58.638	-27.907	1.00	215.12
70	7554 7555	N2 C7	NAG E	243	1.433	57.909	-26.843	1.00	215.12
, ,	7555	O/	NAG E	243	0.428	58.482	-26.182	1.00	215.12

	7556 7557	07 C8	NAG E	243 243	0.027 -0.230	59.633 57.665	-26.423 -25.075	1.00 1.00	215.12 215.12
	7558	C3 ·	NAG E	243	1.685	58.056	-29.247	1.00	215.12
5	7559	03	NAG E	243	0.272	58.105	-29.401	1.00	215.12
,	7560 7561	C4 O4	NAG E	243	2.344	58.866	-30.339	1.00	215.12
	7562	C5	NAG E NAG E	243	1.898	58.318	-31.574	1.00	215.12
	7562 7563	O5	NAG E	243 243	3.883 4.208	58.823	-30.140	1.00	215.12
	7564	C6	NAG E	243	4.206 4.624	59.328 59.699	-28.814	1.00	215.12
10	7565	0 6	NAG E	243	4.268	61.057	-31.116	1.00	215.12
••	7566	C1	MAN E	244	1.748	59.080	-30.933 -32.701	1.00 1.00	215.12
	7567	C2	MAN E	244	2.233	58.170	-33.738	1.00	219.74
	7568	02	MAN E	244	1.708	56.848	-33.490	1.00	219.74 219.74
	7569	C3	MAN E	244	1.963	58.748	-35.107	1.00	219.74
15	7570	O3	MAN E	244	2.548	57.949	-36.119	1.00	219.74
	7571	C4	MAN E	244	0.488	58.983	-35.314	1.00	219.74
•	7572	04	MAN E	244	0.264	59.475	-36.620	1.00	219.74
	7573	C5	MAN E	244	0.038	59.992	-34.253	1.00	219.74
20	7574 7575	O5 C6	MAN E	244	0.282	59.4	-32.908	1.00	219.74
20	7575 7576	O6	MAN E	244	-1.419	60.489	-34.434	1.00	219.74
	7577	C1	MAN E NAG E	244 250	-2.389	59.610	-33.877	1.00	219.74
	7578		NAG E	250 250	12.894 12.331	79.616 80.923	-14.981	1.00	249.69
	7579	N2	NAG E	250	12.351	80.832	-14.392	1.00	249.69
25	7580	C7	NAG E	250	13.100	81.532	-12.946 -12.196	1.00	249.69
	7581	07	NAG E	250	13.967	82.276	-12.673	1.00 1.00	249.69
	7582	C8	NAG E	250	12.966	81.387	-10.683	1.00	249.69 249.69
	7583	СЗ	NAG E	250	10.934	81.188	-14.970	1.00	249.69
20	7584	O3	NAG E	250	10.442	82.440	-14.506	1.00	249.69
30	7585	C4	NAG E	250	10.987	81.183	-16.508	1.00	249.69
	7586	04	NAG E	250	9.667	81.305	-17.032	1.00	249.69
	7587	C5	NAG E	250	11.643	79.872	-17.010	1.00	249.69
	7588 7589	O5	NAG E	250	12.954	79.705	-16.412	1.00	249.69
35	7590	C6 O6	NAG E NAG E	250 250	11.833	79.816	-18.522	1.00	249.69
JJ	7591	C1	NAG E	230 274	12.752 14.635	78.791	-18.892	1.00	249.69
	7592	C2	NAG E	274	13.525	58.650 58.145	0.211 1.158	1.00	249.69
	7593	N2	NAG E	274	13.058	59.230	2.009	1.00 1.00	249.69
	7594	C7	NAG E	274	11.826	59.208	2.513	1.00	249.69 249.69
40	7595	07	NAG E	274	11.030	58.289	2.302	1.00	249.69
	7596	C8	NAG E	274	11.415	60.380	3.387	1.00	249.69
	7597	cз	NAG E	274	14.058	56.984	2.020	1.00	249.69
	7598	03	NAG E	274	12.997	56.422	2.785	1.00	249.69
45	7599	C4	NAG E	274	14.687	55.894	1.134	1.00	249.69
43	7600	O4	NAG E	274	15.298	54.900	1.951	1.00	249.69
	7601 7602	C5 O5	NAG E NAG E	274	15.736	56.513	0.196	1.00	249.69
	7602	C6	NAG E	274 274	15.136 16.324	57.567 EE 500	-0.595	1.00	249.69
	7604	06	NAG E	274 274	17.151	55.500 56.129	-0.775 1.740	1.00	249.69
50	7605	C1	NAG E	335	-13.218	77.155	-1.748 -18.184	1.00	249.69
	7606	C2	NAG E	335	-12.377	77.155 77.952	-17.147	1.00 1.00	248.99
	7607	N2	NAG E	335	-13.025	77.859	-15.850	1.00	248.99 248.99
	7608	C7	NAG E	335	-12.415	77.253	-14.835	1.00	248.99
س س	7609	07	NAG E	335	-11.291	76.751	-14.921	1.00	248.99
55	7610	C8	NAG E	335	-13.169	77.199	-13.517	1.00	248.99
	7611	C3	NAG E	335	-12.169	79.444	-17.498	1.00	248.99
	7612	O3 -	NAG E	335	-11.051	79.949	-16.774	1.00	248.99
	7613	C4	NAG E	335	-11.918	79.636	-18.990	1.00	248.99
60	7614 7615	O4 C5	NAG E	335	-11.812	81.021	-19.294	1.00	248. 99
oo	7616	O5	NAG E	335	-13.079	79.014	-19.748	1.00	248.99
	7617	C6	NAG E NAG E	335 335	-13.060 -12.991	77.584 79.270	-19.562	1.00	248.99
	7618	06	NAG E	335	-14.176		-21.238	1.00	248.99
	7619	C1	NAG E	340	-18.408	79.882 67.970	-21.722 2.712	1.00	248.99
65	7620	C2	NAG E	340	-17.972	66.798	3.606	1.00 1.00	249.69
	7621	N2	NAG E	340	-17.526	65.688	2.783	1.00	249.69 249.69
	7622	C7	NAG E	340	-16.380	65.065	3.055	1.00	249.69
	7623	07	NAG E	340	-15.644	65.372	4.003	1.00	249.69
70	7624	C8	NAG E	340	-15.987	63.917	2.140	1.00	249.69
70	7625	C3	NAG E	340	-19.162	66.374	4.487	1.00	249.69

	7626	O 3	NAG E	340	-18.769	65.355	5.395	1.00	249.69
	7627	C4	NAG E	340	-19.704	67.580	5.273	1.00	249.69
	7628	O4 [*]	NAG E	340	-20.884	67.199	5.975	1.00	249.69
_	7629	C5	NAG E	340	-20.011	68.748	4.305	1.00	249.69
5	7630	O5	NAG E	340	-18.836	69.073	3.520	1.00	249.69
	7631	C6	NAG E	340	-20.450	70.028	5.000	1.00	249.69
	7632	O6	NAG E	340	-20.520	71.112	4.081	1.00	249.69
	7633	C1	NAG E	366	-13.236	53.354	-17.338	1.00	200.99
	7634	C2	NAG E	366	-12.501	52.697	-18.503	1.00	200.99
10	7635	N2	NAG E	366	-12.267	53.689	-19.539	1.00	200.99
	7636	C7	NAG E	366	-11.142	54.405	-19.544	1.00	200.99
	7637	07	NAG E	366	-10.251	54.258	-18.697	1.00	200.99
	7638	C8	NAG E	366	-10.974	55.435	-20.659	1.00	200.99
	7639	СЗ	NAG E	366	-13.344	51.559	-19.064	1.00	200.99
15	7640	O3	NAG E	366	-12.589	50.845	-20.024	1.00	200.99
	7641	C4	NAG E	366	-13.814	50.601	-17.968	1.00	200.99
	7642	04	NAG E	366	-14.809	49.714	-18.523	1.00	200.99
	7643	C5	NAG E	366	-14.427	51.387	-16.796	1.00	200.99
	7644	O 5	NAG E	366	-13.511	52.389	-16.333	1.00	200.99
20	7645	C6	NAG E	366	-14.780	50.532	-15.594	1.00	200.99
	7646	O 6	NAG E	366	-15.500	51.287	-14.628	1.00	200.99
	7647	C1	NAG E	367	-14.595	48.351	-18.366	1.00	248.88
	7648	C2	NAG E	367	-15.915	47.598	-18.528	1.00	248.88
0.5	7649	N2	NAG E	367	-16.897	48.084	-17.575	1.00	248.88
25	7650	C7	NAG E	367	-17.964	48.748	-18.004	1.00	248.88
	7651	07	NAG E	367	-18.175	48.977	-19.195	1.00	248.88
	7652	C8	NAG E	367	-18.948	49.229	-16.950	1.00	248.88
	7653	C3	NAG E	367	-15.646	46.102	-18.325	1.00	248.88
20	7654	O 3	NAG E	367	-16.851	45.362	-18.485	1.00	248.88
30	7655	C4	NAG E	367	-14.602	45. 63 1	-19.346	1.00	248.88
	7656	O4	NAG E	367	-14.273	44.271	-19.099	1.00	248.88
	7657	C 5	NAG E	367	-13.334	46.502	-19.256	1.00	248.88
	7658	O 5	NAG E	367	-13.668	47.911	-19.373	1.00	248.88
25	7659	C6	NAG E	367	-12.347	46.188	-20.363	1.00	248.88
35	7660	O 6	NAG E	367	-12.226	47.271	-21.276	1.00	248.88

Table 7. Atomic coordinates of PhFceRIa₁₋₁₇₆, Form M2

	ATOM NUMBER	ATOM TYPE	RESIDUE		_ <u>x</u> _	<u>_Y_</u>	_Z	<u>000</u>	B
	1	СВ	VAL A	1	54.132	-20.714	8.499	1.00	470.40
5	2	CG1	VAL A	1	52,843	-21.062	7.774	1.00	178.10 175.86
	3	CG2	VAL A	1	54.598	-21.899	9.342	1.00	170.07
	4 5	C O	VAL A VAL A	1	55.044	-18.854	6.922	1.00	182.13
	6	N	VAL A VAL A	1	54.219	-18.626	6.045	1.00	181.45
10	7	CA	VAL A	i	56.560 55.237	-20.445 -20.291	8.067 7.470	1.00 1.00	185.40
	8	N	PRO A	2	55.807	-17.881	7.435	1.00	181.27 180.05
	9	CD	PRO A	2	55.929	-17.840	8.889	1.00	177.25
	10	CA	PRO A	2	55.680	-16.493	6.950	1.00	173.64
15	11 12	CB CG	PRO A PRO A	2	56.618	-15.752	7.867	1.00	173.09
	13	Č	PRO A	2 2	56.407 55.836	-16.439 -16.175	9.184 5.460	1.00	173.72
	14	0	PRO A	2	55.605	-15.044	5.015	1.00 1.00	167.05 168.35
	15	N	GLN A	2	56.252	-17.165	4.696	1.00	154.29
20	16	CA	GLN A	3	56.695	-17.039	3.302	1.00	144.07
20	17 18 .	CB CG	GLN A GLN A	3	56.716	-18.462	2.775	1.00	152.72
	19	CD	GLN A GLN A	3 3	57.593 58.812	-19.352 -18.642	3.656	1.00	159.56
	20	OE1	GLN A	3	59.151	-17.549	4.253 3.808	1.00 1.00	162.34
	21	NE2	GLN A	3	59.600	-19.090	5.219	1.00	167.23 166.20
25	22	С	GLN A	3	56.117	-15.992	2.286	1.00	134.57
	23	0	GLN A	3	56.663	-15.988	1.196	1.00	145.79
	24 25	N CA	LYS A	4	55.146	-15,111	2.520	1.00	114.68
	26	CB	LYS A LYS A	4	54.768 53.529	-14.237 -14.805	1.357	1.00	91.89
30	27	CG	LYS A	4	52.415	-15.272	0.655 1.595	1.00 1.00	93.44
	28	CD	LYS A	4	51.061	-15.271	0.914	1.00	116.31 123.93
	29	CE	LYS A	4	50.072	-16.156	1.643	1.00	131.64
	30	NZ	LYS A	4	49.049	-16.742	0.732	1.00	135.93
35	31 32	C O	LYS A LYS A	4	54.546 54.000	-12.760	1.718	1.00	72.33
20	33	Ň	PRO A	5	54.002 54.961	-12.486 -11.818	2.790 0.861	1.00	69.94
	34	CD	PRO A	5	55.670	-12.005	-0.413	1.00 1.00	46.80 34.03
	3 5	CA	PRO A	5 5	54.807	-10.400	1.180	1.00	35.08
40	36	CB	PRO A	5	55.351	-9.708	-0.066	1.00	27.27
40	37 38	ca c	PRO A	5	56.350	-10.674	-0.591	1.00	18.92
	39	ŏ	PRO A PRO A	5 5	53.320 52.473	-10.124 -10.945	1.371	1.00	41.36
	40	Ň	LYS A	6	52.988	-8.970	1.030 1.915	1.00 1.00	59.20 45.12
	41	CA	LYS A	6	51.591	-8.644	2.112	1.00	58.01
45	42	CB	LYS A	6	51.207	-8.907	3.570	1.00	31.24
	43	CG	LYS A	6	49.726	-8.775	3.844	1.00	63.36
	44 45	CD CE	LYS A LYS A	6	49.203	-10.005	4.566	1.00	81.81
	46	NZ	LYS A LYS A	6 6	47.699 47.156	-9.917 -11.172	4.797 5.406	1.00	83.24
50	47	Ċ	LYS A	6	51.392	-7.177	1.734	1.00 1.00	80.30 61.99
	48	0	LYS A	6	51.822	-6.280	2.460	1.00	80.08
	49	N.	VAI A	7	50.773	-6.936	0.583	1.00	46.06
	50 51	CA	VAL A	7	50.542	-5.574	0.153	1.00	39.39
55	51 52	CB CG1	VAL A VAL A	7 7	49.937 49.551	-5.529 4.007	-1.254	1.00	45.45
	53	CG2	VAL A	7	50.947	-4.097 -6.057	-1.603 -2.270	1.00	49.77
	54	C	VAL A	7	49.594	-4.890	1.125	1.00 1.00	22.27 44.09
	55	0	VAL A	7	48.558	-5.446	1.493	1.00	37.53
60	56	N	SER A	8	49.970	-3.686	1.546	1.00	52.74
oo	57 58	CA CB	SER A	8	49.162	-2.909	2.474	1.00	53.44
	59	OG	SER A SER A	8 8	49.936 50.799	-2.627 -1.517	3.752	1.00	61.38
	60	C	SER A	8	48.886	-1.517 -1.598	3.558 1.772	1.00 1.00	88.92 51.41
~	61	0	SER A	8	49.698	-1.134	0.963	1.00	45.35
65	62	N	LEU A	9	47.753	-0.988	2.080	1.00	44.36
	63 64	CA	LEU A	9	47.422	0.260	1.422	1.00	49.82
	04	CB	LEU A	9	46.027	0.193	0.778	1.00	64.30

	65 66	CG CD1	LEU A LEU A	9 ·	45.511 44.236	-1.067	0.680	1.00	48.97
	67	CD2	LEU A	9	46.536	-0.713 -1.600	-0.646 -0.898	1.00	42.71
_	68	C	LEU A	9	47.429	1.408	2.405	1.00 1.00	20.50
5	69	0	LEU A	9	47.003	1.263	3.551	1.00	39.97 31.04
	70 71	N CA	ASN A	10	47.892	2.557	1.937	1.00	39.17
	72	CA CB	ASN A ASN A	10 10	47.888 49.249	3.747	2.758	1.00	38.83
	73	ČĞ	ASN A	10	49.281	3.992 5.278	3.387 4.188	1.00	56.48
10	74	OD1	ASN A	10	48.500	5.445	5.135	1.00 1.00	70.12
	75	ND2	ASN A	10	50.169	6.205	3.807	1.00	58.68 68.79
	76 77	C	ASN A	10	47.518	4.957	1.909	1.00	31.34
	78	0 N	ASN A PRO A	10	48.302	5.400	1.040	1.00	26.78
15	79	CD	PRO A	11 11	46.305 45.988	5.494 6.856	2.124	1.00	9.37
	80	CA	PRO A	11	45.313	5.030	1.655 3.102	1.00 1.00	13.93
	81	CB	PRO A	11	44.263	6.137	3.082	1.00	18.39 26.39
	82	ČG	PRO A	11	45.107	7.388	2.763	1.00	26.16
20	83 84	C O	PRO A PRO A	11	44.718	3.662	2.745	1.00	29.16
20	85	Ň	PRO A	11 12	44.619 44.277	3.300	1.579	1.00	42.47
	86	CD	PRO A	12	44.139	2.911 3.482	3. 7 59 5.107	1.00	29.44
	87	CA	PRO A	12	43.673	1.578	3.725	1.00 1.00	42.51 43.05
25	88	CB	PRO A	12	43.049	1.454	5.115	1.00	41.74
23	89 90	CG	PRO A	12	43.957	2.251	5.951	1.00	59.93
	91	Ö	PRO A PRO A	12 12	42.625	1.358	2.645	1.00	51.72
	92	Ň	TRP A	13	42.384 41.985	0.223 2.444	2.220 2.231	1.00	61.36
20	93	CA	TRP A	13	40.926	2.405	1.232	1.00 1.00	52.05 45.67
30	94	CB	TRP A	13	40.423	3.818	1.033	1.00	48.38
	95 96	CG	TRP A	13	40.354	4.497	2.343	1.00	49.00
	97	CD2 CE2	TRP A TRP A	13 13	39.731	3.991	3.519	1.00	33.76
	98	CE3	TRP A	13	39.943 39.013	4.934 2.827	4.542 3.809	1.00 1.00	31.11
35	99	CD1	TRP A	13	40.908	5.693	2.685	1.00	30.50 46.06
	100	NE1	TRP A	13	40.667	5.962	4.005	1.00	48.28
	101 102	CZ2 CZ3	TRP A TRP A	13	39.463	4.755	5.837	1.00	28.30
	103	CH2	TRP A	13 13	38.536 38.764	2.646 3.610	5.102	1.00	40.23
40	104	C	TRP A	13	41.348	1.802	6.100 -0.087	1.00 1.00	32.97 47.41
	105	0	TRP A	13	42.162	2.382	-0.809	1.00	45.41
	106 107	N CA	ASN A ASN A	14	40.796	0.627	-0.386	1.00	52.08
	108	CB	ASN A	14 14	41.102 40.891	-0.084 -1.578	-1.622	1.00	50.75
45	109	CG	ASN A	14	39.442	-1.920	-1.434 -1.257	1.00 1.00	45.92
	110	OD1	ASN A	14	38.790	-1.435	-0.331	1.00	58.48 59.48
	111	ND2	ASN A	14	38.916	-2.747	-2.153	1.00	60.88
	112 113	C	ASN A ASN A	14	40.171	0.433	-2.716	1.00	49.24
50	114	Ň	ARG A	15	40.280 39.238	0.060 1.284	-3.881	1.00	55.28
	115	CA	ARG A	15	38.310	1.895	-2.317 -3.250	1.00 1.00	40.77 33.20
	116	CB	ARG A	15	36.875	1.556	-2.879	1.00	21.25
	117 118	CG CD	ARG A	15	36.724	0.305	-2.085	1.00	42.18
55	119	NE	ARG A ARG A	15 15	35.250 34.488	0.125	-1.761	1.00	35.91
	120	CZ	ARG A	15	33.194	-0.087 0.157	-2.981 -3.092	1.00	10.90
	121	NH1	ARG A	15	32.538	0.624	-2.051	1.00 1.00	35.38 33.36
	122 123	NH2	ARG A	15	32.563	-0.078	-4.231	1.00	59.41
60	124	C	ARG A ARG A	15	38.518	3.406	-3.108	1.00	32.71
	125	Ň	ILE A	15 16	38.262 38.965	3.995 4.051	-2.058	1.00	18.86
	126	CA	ILE A	16	39.191	5.470	-4.168 -4.083	1.00 1.00	25.83
	127	CB	ILE A	16	40.666	5.698	-4.000	1.00	22.32 4.67
65	128 129	CG2	ILE A	16	41.229	4.810	-2.957	1.00	24.87
0 5	130	CG1 CD1	ILE A ILE A	16 16	41.319	5.326	-5.326	1.00	5.49
•	131	C C	ILE A	16 16	42.840 38.620	5.449 6.262	-5.311 -5.252	1.00	5.72
	132	0	ILE A	16	38.407	5.729	-5.253 -6.332	1.00 1.00	27.38 50.75
70	133	N	PHE A	17	38.380	7.545	-5.024	1.00	50.75 29.15
70	134	CA	PHE A	17	37.877	8.447	-6.047	1.00	14.06
				-		•			

	135 136	CB CG	PHE A	17. 17	37.408 36.041	9.741 9.655	-5.400 -4.819	1.00 1.00	10.31 5.03
	137	CD1	PHE A	17	35.697	10.396	-3.697	1.00	17.85
5	138 139	CD2 · CE1	PHE A PHE A	17	35.071	8.885	-5.431	1.00	6.30
-	140	CE2	PHE A	17 17	34.385 33.743	10.376 8.853	-3.190 -4.934	1.00	28.74
	141	CZ	PHE A	17	33.399	9.598	-3.817	1.00 1.00	28.88
	142	С	PHE A	17	38.975	8.769	-7.051	1.00	19.77 25.28
10	143	0	PHE A	17	40.159	8.770	-6.717	1.00	27.78
10	144 145	N	LYS A	18	38.567	9.041	-8.283	1.00	38.02
	145	CA CB	LYS A LYS A	18 18	39.502 38.736	9.379	-9.346	1.00	41.11
	147	ČG	LYS A	18	39.565	9.665 10.297	-10.645 -11.754	1.00	37.45
	148	CD	LYS A	18	38.672	10.698	-12.919	1.00 1.00	38.42 71.68
15	149	CE	LYS A	18	39.477	11.290	-14.078	1.00	82.18
	150	NZ	LYS A	18	40.148	12.572	-13.720	1.00	90.91
	151 152	C O	LYS A LYS A	18	40.280	10.612	-8.932	1.00	42.58
	153	N	LYS A GLY A	18 19	39.707 41.582	11.549 10.607	-8.376	1.00	50.79
20	154	CA	GLY A	19	42.389	11.763	-9.193 -8.843	1.00	38.08
	155	C	GLY A	19	42.987	11.754	-0.043 -7.445	1.00 1.00	50.88
	156	0	GLY A	19	43.838	12.600	-7.117	1.00	51.07 53.98
	157	N	GLU A	20	42.537	10.820	-6.609	1.00	35.00
25	158 159	CA	GLU A	20	43.081	10.712	-5.266	1.00	30.62
23	160	CB CQ	GLU A GLU A	20	42.113	9.993	-4.338	1.00	17.69
	161	CD	GLU A	20 20	40.753 39.951	10.651 10.197	-4.261	1.00	52.43
	162	OE1	GLU A	20	39.832	8.970	-3.050 -2.84 2	1.00 1.00	59.33
	163	OE2	GLU A	20	39.437	11.064	-2.306	1.00	67.80 52.52
30	164	Ç	GLU A	20	44.402	9.953	-5.301	1.00	40.13
	165	0	GLU A	20	44.789	9.367	-6.321	1.00	29.35
	166 167	N CA	ASN A ASN A	21	45.089	9.958	-4.171	1.00	39.02
	168	CB	ASN A	21 21	46.375 47.390	9.303 10.310	-4.083	1.00	35.97
35	169	CG	ASN A	21	47.721	11.379	-3.549 -4.569	1.00 1.00	52.23
	170	OD1	ASN A	21	48.190	11.032	-5.657	1.00	60.60 71.53
	171	ND2	ASN A	21	47.493	12.658	-4.253	1.00	51.64
	172 173	C	ASN A	21	46.307	8.066	-3.204	1.00	39.75
40	173	0 N	ASN A VAL A	21	45.377	7.916	-2.390	1.00	35.49
10	175	ČA	VAL A	22 22	47.263 47.311	7.160 5.934	-3.393	1.00	30.65
	176	CB	VAL A	22	46.241	4.918	-2.597 -3.040	1.00	25.06
	177	CG1	VAL A	22	46.606	4.337	-4.418	1.00 1.00	31.80 36.39
15	178	CG2	VAL A	22	46.083	3.825	-1.985	1.00	5.71
45	179	C	VAL A	22	48.678	5.312	-2.761	1.00	33.39
	180 181	0 N	VAL A THR A	22	49.291	5.422	-3.833	1.00	34.28
	182	GA CA	THR A	23 23	49.168 50.499	4.669 4.073	-1.704	1.00	44.00
	183	CB	THR A	23	51.497	4.815	-1.755 -0.829	1.00 1.00	47.12
50	184	OG1	THR A	23	51.516	6.216	-1.138	1.00	48.39 51.20
	185	CG2	THR A	23	52.903	4.243	-1.015	1.00	33.54
	186	C	THR A	23	50.508	2.610	-1.356	1.00	39.06
	187 188	O N	THR A LEU A	23	50.146	2.261	-0.228	1.00	40.82
55	189	CA CA	LEU A	24 24	50.920	1.758	-2.286	1.00	36.12
	190	CB	LEU A	24	50.982 50.773	0.337 -0.471	-2.012 -3. 29 4	1.00	42.23
	191	CG	LEU A	24	49.429	-0.222	-3.968	1.00 1.00	36.69 33.10
	192	CD1	LEU A	24	49.240	-1.186	-5.117	1.00	50.66
60	193	CD2	LEU A	24	48.321	-0.391	-2.938	1.00	31.21
w	194 195	C O	LEU A	24	52.352	0.044	-1.444	1.00	42.69
	196	N	THR A	24 25	53.364	0.492	-1.991	1.00	30.60
	197	CA	THR A	25 25	52.392 53.667	-0.704 -1.046	-0.346	1.00	52.44
	198	CB	THR A	25	53.806	-0.422	0.263 1.652	1.00 1.00	58.07 62.06
65	199	OG1	THR A	25	53.423	0.958	1.601	1.00	59.04
	200	CG2	THR A	25	55.252	-0.519	2.115	1.00	57.89
	201 202	C O	THR A	25	53.820	-2.557	0.373	1.00	58.45
	203	N	THR A	25 26	52.874 55.015	-3.261	0.754	1.00	57.55
70	204	CA	CYS A	26 26	55.015 55.334	-3.039 -4.465	0.035	1.00	48.91
	-	•			~	⊸7.700	0.061	1.00	53.25

		_							
	205	C	CYS A	26	56.187	-4.793	1.272	1.00	65.21
	206	0	CYS A	26	57.370	-4.444	1.305	1.00	62.05
	207 208	CB: SG	CYS A CYS A	26	56.103	-4.833	-1.201	1.00	58.57
5	209	N N	ASN A	26 27	56.163	-6.602 5.400	-1.640	1.00	76.24
	210	ČA	ASN A	27 27	55.594 56.319	-5.489 -5.806	2.266	1.00	76.22
	211	CB	ASN A	27	55.742	-5.025	3.490	1.00	94.33
	212	CG	ASN A	27	54.369	-5.518	4.670	1.00	99.45
	213	OD1	ASN A	27	53.835	-6.457	5.080 4.490	1.00	114.67
10	214	ND2	ASN A	27	53.792	-4.886	6.095	1.00	126.31
	215	С	ASN A	27	56.288	-7.302	3.775	1.00 1.00	113.87
	216	0	ASN A	27	55.477	-8.061	3.274	1.00	96.08
	217	N	GLY A	28	57. 22 7	-7.729	4.653	1.00	101.25 92.99
	218	CA	GLY A	28	57.316	-9.125	5.042	1.00	93.67
15	219	С	GLY A	28	58.420	-9.329	6.058	1.00	97.85
	220	0	GLY A	28	59.153	-8.393	6.368	1.00	107.57
	221	N	ASN A	29	58.544	-10.542	6.583	1.00	96.86
	222	CA	ASN A	29	59.581	-10.846	7.561	1.00	94.84
20	223 224	CB	ASN A	29	59.517	12.310	7.954	1.00	99.10
20	224 225	CG OD1	ASN A	29	58.106	-12.811	8.040	1.00	116.98
	226	ND2	ASN A	29	57.352	-12.453	8. 948	1.00	116.13
	227	C	ASN A ASN A	29	57. 72 6	-13.631	7.077	1.00	132.36
	228	ŏ	ASN A	29	60.941	-10.562	6.954	1.00	97.30
25	229	Ň	ASN A	29 30	61.245	-11.011	5.846	1.00	100.89
	230	ĊA	ASN A	30	61.761 63.090	-9.821 -9.479	7.683	1.00	95.34
	231	CB	ASN A	30	63.751	-8.483	7. 209 8.165	1.00	100.29
	232	CG	ASN A	30	62.971	-7.188	8.288	1.00	108.20
	233	OD1	ASN A	30	62.798	-6.453	7.314	1.00 1.00	117.57
30	234	ND2	ASN A	30	62.494	-6.900	9.498	1.00	118.50 125.45
	235	С	ASN A	30	63.979	-10.709	7.086	1.00	99.61
	236	0	ASN A	30	65.174	-10.573	6.812	1.00	111.39
	237	N	PHE A	31	63.407	-11.903	7.278	1.00	87.84
25	238	CA	PHE A	31	64.181	-13.146	7.201	1.00	71.61
35	239	СВ	PHE A	31	63.288	-14.344	6.949	1.00	63.53
	240	CG	PHE A	31	63.993	-15.645	7.148	1.00	71.95
	241 242	CD1	PHE A	31	64.017	-16.257	8.395	1.00	79.52
	242	CD2 CE1	PHE A	31	64.687	-16.234	6.099	1.00	82.44
40	244	CE2	PHE A PHE A	31	64.724	-17.444	8.595	1.00	77.29
	245	CZ	PHE A	31 31	65.400	-17.420	6.284	1.00	89.06
	246	č	PHE A	31	65.420	-18.025	7.538	1.00	83.28
	247	ŏ	PHE A	31	65.252 66.452	-13.102 -13.207	6.111	1.00	69.17
	248	Ň	PHE A	32	64.809	-13.207	6.393 4.865	1.00	84.06
45	249	CA	PHE A	32	65.736	-12.851	3.750	1.00	59.43
	250	СВ	PHE A	32	65.255	-13.673	2.565	1.00 1.00	52.65
	251	CG	PHE A	32	65.585	-15.134	2.659	1.00	41.66
	252	CD1	PHE A	32	64.584	-16.073	2.907	1.00	47.56 44.68
50	253	CD2	PHE A	32	66.897	-15.575	2.492	1.00	51.53
50	254	CE1	PHE A	32	64.883	-17,433	2.989	1.00	43.51
	255	CE2	PHE A	32	67.208	-16.938	2.580	1.00	51.46
	256	CZ	PHE A	32	66.196	-17.866	2.824	1.00	52.70
	257	C	PHE A	32	65.794	-11.375	3.345	1.00	58.83
55	258	0	PHE A	32	64.773	-10 .69 8	3.278	1.00	56.92
23	259 260	N	GLU A	33	66.990	-10.875	3.080	1.00	62.55
	261	CA CB	GLU A	33	67.152	-9.482	2.695	1.00	69.28
	262	CG	GLU A	33	68.640	-9.164	2.586	1.00	88.52
	263	· CD	GLU A GLU A	33	69.291	-8.758	3.901	1.00	69.46
60	264	OE1	GLU A	33 33	70.782	-8.585 0.007	3.753	1.00	84.74
	265	OE2	GLU A	33	71.225 71.516	-8.087	2.697	1.00	88.47
	266	č	GLU A	33	66.436	-8.945 -9.106	4.693	1.00	105.94
	267	ŏ	GLU A	33	66.268	-9.936	1.391	1.00	64.49
	268	N	VAL A	34	66.045	-7.837	0.490 1.292	1.00	58.36
65	269	CA	VAL A	34	65.345	·7.329	0.123	1.00	53.30
	270	СВ	VAL A	34	63.852	-7.116	0.123	1.00 1.00	45.11 49.71
	271	CG1	VAL A	34	63.143	-6.517	-0.760	1.00	48.71 64.13
	272	CG2	VAL A	34	63.207	-8.418	0.846	1.00	12.46
70	273	Č	VAL A	34	65.902	-5.992	-0.379	1.00	53.63
70	274	0	VAL A	34	65.671	-4.944	0.233	1.00	61.37
									V1.07

	275	N	SER A	35-	66.614	-6.020	-1.499	1.00	49.22
	276	CA	SER A	35	67.155	-4.790	-2.063	1.00	59.53
	277	CB:	SER A	35	68.650	-4.931	-2.345	1.00	70.72
_	278	OG '	SER A	35	68.886	-5.671	-3.532	1.00	78.30
5	279	C	SER A	35	66.438	-4.442	-3.362	1.00	65.71
	280	0	SER A	35	66.894	-3.576	-4.106	1.00	79.59
	281	N	SER A	36	65.325	-5.122	-3.631	1.00	71.64
	282	CA	SER A	36	64.546	-4.889	-4.849	1.00	68.57
	283	CB	SER A	36	65.307	-5.378	-6.084	1.00	
10	284	OG	SER A	36	65.260	-6.790	-6.186	1.00	72.44
	285	Ċ.	SER A	36	63,197	-5.593	-4.805		79.50
	286	ŏ	SER A	36	63.070	-6.691	-4.265	1.00	63.12
	287	Ň	THR A	37	62.189	-4.961		1.00	64.24
	288	ČA	THR A	37	60.850		-5.391	1.00	60.88
15	289	CB	THR A			-5.529	-5.417	1.00	47.23
13	290	OG1		37	59.864	-4.621	-4.687	1.00	45.28
			THR A	37	60.421	-4.251	-3.420	1.00	61.45
	291	CG2	THR A	37	58.521	-5.336	-4.477	1.00	29.55
	292	C	THR A	37	60.363	-5.712	-6.854	1.00	48.75
20	293	0	THR A	37	60.992	-5.240	-7.809	1.00	46.94
20	294	N -	LYS A	38	59.244	-6.406	-7.002	1.00	44.37
	295	ÇA	LYS A	38	58.658	-6.655	-8.308	1.00	27.76
	296	CB	LYS A	38	58.820	-8.117	-8.693	1.00	41.96
	297	CG	LYS A	38	59.620	-8.368	-9.929	1.00	34.76
~ ~	298	CD	LYS A	38	61.033	-7.877	-9.768	1.00	57.35
25	299	CE	LYS A	38	61.944	-8.534	-10.793	1.00	65.86
	300	NZ	LYS A	38	61.835	-10.029	-10.698	1.00	34.19
	301	С	LYS A	38	57.184	-6.351	-8.160	1.00	39.95
	302	0	LYS A	38	56.489	-6.975	-7.341	1.00	37.00
	303	N	TRP A	39	56.705	-5.384	-8.934	1.00	
30	304	CA	TRP A	39	55.292	-5.012	-8.878		51.66
	305	CB	TRP A	39	55.130	-3.498		1.00	46.32
	306	CG	TRP A	39	55.477	-3.023	-8.736 7.330	1.00	37.04
	307	CD2	TRP A	39	54.615		-7.372	1.00	41.46
	308	CE2	TRP A	39		-3.022	-6.233	1.00	14.22
35	309	CE3	TRP A		55. 360	-2.534	-5.141	1.00	5.00
55	310	CD1		39	53.284	-3.389	-6.025	1.00	27.18
			TRP A	39	56.685	-2.548	-6.940	1.00	38.68
	311	NE1	TRP A	39	56.622	-2.252	-5. 597	1.00	29.64
	312	CZ2	TRP A	39	54.819	-2.396	-3.864	1.00	25.70
40	313	CZ3	TRP A	39	52.745	-3.253	-4.742	1.00	38.07
40	314	CH2	TRP A	39	53.514	-2.761	-3.683	1.00	26.72
	315	Ç	TRP A	39	54.531	-5.501	-10.102	1.00	35.61
	316	0	TRP A	39	55.080	, -5 <i>.</i> 587	-11.209	1.00	19.21
	317	Ņ	PHE A	40	53.266	- 5. 83 3	-9.898	1.00	11.64
4 ~	318	CA	PHE A	40	52.480	-6.327	-10.994	1.00	6.70
45	319	СВ	PHE A	40	52.340	-7.853	-10.899	1.00	19.61
	320	CG	PHE A	40	53. 64 4	-8.595	-11.029	1.00	22.54
	321	CD1	PHE A	40	54.445	-8.807	-9.935	1.00	38.72
	322	CD2	PHE A	40	54.100	-9.019	-12.262	1.00	33.22
	323	CE1	PHE A	.40	55.673	-9.409	-10.067	1.00	29.68
50	324	CE2	PHE A	40	55.334	-9.625	-12.395	1.00	36.71
	325	CZ	PHE A	40	56.117	-9.818	-11.296	1.00	35.88
	326	C	PHE A	40	51.108	-5.687	-11.031	1.00	37.09
	327	0	PHE A	40	50.263	-5.931	-10.145	1.00	42.94
	328	N	HIS A	41	50.902	-4.846	-12.046		
55	329	CA	HIS A	41	49.604	-4.207	-12.245	1.00	41.78
	330	СВ	HIS A	41	49.734	-2.831		1.00	41.13
	331	ČĠ	HIS A	41		-2.055 -2.055	-12.878	1.00	45.29
	332	CD2	HIS A		48.457		-12.857	1.00	22.20
	333	ND1		41	48.178	-0.784	-13.225	1.00	33.03
60	334	CE1		41	47.288	-2.576	-12.347	1.00	36.74
00	335	NE2		41	46.341	-1.656	-12.396	1.00	31.11
			HIS A	41	46.856	-0.558	-12.924	1.00	55.47
	336	C	HIS A	41	48.903	-5.131	-13.215	1.00	29.92
	337	0	HIS A	41	49.468	-5.495	-14.246	1.00	19.98
65	338	N	ASN A	42	47.688	-5.532	-12.876	1.00	26.06
O)	339	CA	ASN A	42	46.968	-6.458	-13.730	1.00	33.33
	340	CB	ASN A	42	46.265	-5.680	-14.834	1.00	17.02
	341	CG	ASN A	42	45.045	-4.956	-14.334	1.00	32.02
	342	OD1	ASN A	42	44.490	-5.335	-13.274	1.00	29.56
70	343	ND2	ASN A	42	44.618	-3.945	-15.101	1.00	13.43
70	344	С	ASN A	42	47.924	-7.520	-14.333	1.00	38.30
									-0.00

-	^	•
-3	Z	D-

		_							
	345	0	ASN A	42 -	47.954	-7.738	-15.548	1.00	35.70
	346	N _.	GLY A	43	48.723	-8.150	-13.476	1.00	39.92
	347	CA:	GLY A	43	49.640	-9.182	-13.926	1.00	32.70
_	348	Ç .	GLY A	43	50.880	-8.741	-14.686	1.00	36.33
5	349	0	GLY A	43	51.786	-9.544	-14.891	1.00	40.53
	350	Ň	SER A	44	50.946	-7.489	-15.117	1.00	34.42
	351	CA	SER A	44	52.124	-7.048	-15.862	1.00	44.42
	352	СВ	SER A	44	51.738	-6.05 5	-16.957	1.00	57.35
	353	OG	SER A	44	50.928	-6.677	-17.942	1.00	77.66
10	354	С	SER A	44	53.128	-6.402	-14.947	1.00	42.83
	355	0	SER A	44	52.755	-5.629	-14.072	1.00	48.20
	356	N	LEU A	45	54.404	-6.713	-15.153	1.00	46.97
	357	CA	LEU A	45	55.472	-6.160	-14.322	1.00	46.50
. ~	358	CB	LEU A	45	56.819	-6.805	-14.665	1.00	33.26
15	359	CG	LEU A	45	58.045	-6.173	-13.999	1.00	34.18
	360	CD1	LEU A	45	57.912	-6.233	-12.476	1.00	58.24
	361	CD2	LEU A	45	59.287	-6.896	-14.445	1.00	39.00
	362	С	LEU A	45	55.581	-4.658	-14.501	1.00	46.94
	363	0	LEU A	45	55.627	-4.180	-15.611	1.00	34.79
20	364	N	SER A	46	55.612	-3.922	-13.400	1.00	60.24
	365	CA	SER A	46	55.721	-2.478	-13.456	1.00	54.99
	366	CB	SER A	46	55.040	-1.857	-12.240	1.00	58.08
	367	OG	SER A	46	55.175	-0.446	-12.254	1.00	81.72
0.5	368	С	SER A	46	57.191	-2.132	-13.442	1.00	58.15
25	369	0	SER A	46	58.023	-2.965	-13.100	1.00	70.14
	370	N	GLU A	47	57.513	-0.902	-13.819	1.00	57.45
	371	CA	GLU A	47	58.900	-0.462	-13.822	1.00	65.18
	372	CB	GLU A	47	59.070	0.748	-14.735	1.00	75.20
••	373	CG	GLU A	47	58.981	0.417	-16.207	1.00	98.71
30	374	CD	GLU A	47	59.119	1.648	-17.075	1.00	118.62
	375	OE1	GLU A	47	58.207	2.505	-17.038	1.00	131.08
	376	OE2	GLU A	47	60.140	1.761	-17.788	1.00	126.76
	377	С	GLU A	47	59.352	-0.109	-12.408	1.00	63.59
~ ~	378	0	GLU A	47	60.551	-0.117	-12.108	1.00	67.24
35	379	N	GLU A	48	58.382	0.193	-11.546	1.00	53.32
	380	CA	GLU A	48	58.653	0.539	-10.156	1.00	55.75
	381	CB	GLU A	48	57.343	0.802	-9.422	1.00	58.11
	382	CG	GLU A	48	57.530	1.166	-7.964	1.00	86.91
	383	CD	GLU A	48	58.235	2.501	-7.781	1.00	104.21
40	384	OE1	GLU A	48	57.545	3.548	-7.752	1.00	116.45
	385	OE2	GLU A	48	59.483	2.499	-7.681	1.00	107.36
	386	С	GLU A	48	59.403	-0.581	-9.442	1.00	57.10
	387	0	GLU A	48	59.016	-1.744	-9.518	1.00	64.00
	388	N	THR A	49	60.471	-0.230	-8.735	1.00	54.72
45	389	CA	THR A	49	61.253	-1.238	-8.024	1.00	63.14
	390	CB	THR A	49	62.646	-1.380	-8.647	1.00	63.41
	391	OG1	THR A	49	62.980	-0.174	-9.345	1.00	62.51
	392	CG2	THR A	49	62.677	-2.552	-9.603	1.00	64.13
50	393	С	THR A	49	61.415	-1.015	-6.521	1.00	62.86
50	394	0	THR A	49	62.066	-1.806	-5.839	1.00	69.10
	395	N	ASN A	50	60.821	0.052	-6.003	1.00	54.53
	396	CA	ASN A	50	60.918	0.341	-4.580	1.00	61.75
	397	CB	ASN A	50	60.864	1.860	-4.331	1.00	76.64
ہے ہے	398	CG	asn a	50	61.974	2.623	-5.065	1.00	80.85
55	399	OD1	ASN A	50	63.136	2.211	-5.063	1.00	73.80
	400	ND2	.SN A	50	61.615	3.745	-5.686	1.00	83.17
	401	С	ASN A	50	59.795	-0.365	-3.827	1.00	60.45
	402	0	ASN A	50	58.718	-0.579	-4.361	1.00	64.31
	403	N	SER A	51	60.053	-0.723	-2.579	1.00	64.42
60	404	CA	SER A	51	59.067	-1.417	-1.767	1.00	69.19
	405	СВ	SER A	51	59.649	-1.690	-0.383	1.00	83.18
	406	OG	SER A	51	60.136	-0.498	0.207	1.00	98.67
	407	C	SER A	51	57.757	-0.651	-1.633	1.00	72.43
	408	0	SER A	51	56.779	-1.160	-1.076	1.00	75.57
65	409	N	SER A	52	57.738	0.577	-2.138	1.00	72.75
	410	CA	SER A	52	56.535	1.391	-2.069	1.00	72.90
	411	СВ	SER A	52	56.766	2.600	-1.165	1.00	77.27
	412	OG	SER A	52	57.143	2.182	0.137	1.00	104.21
	413	C	SER A	52	56.106	1.858	-3.449	1.00	69.39
70	414	0	SER A	52	56.806	2.617	-4.114	1.00	68.69
									20.00

	415	N	LEU A	53 [.]	54.950	1.376	.2 002	4.00	
	416	CA	LEU A	53	54.405	1.754	-3.883 -5.176	1.00 1.00	70.92 66.04
	417 418	CB ·	LEU A	53	53.747	0.542	-5.841	1.00	64.62
5	419	CD1	LEU A LEU A	53 53	52.954 53.761	0.809	-7.120	1.00	57.82
_	420	CD2	LEU A	53	52.593	1.661 -0.504	-8.068 -7.758	1.00 1.00	53.42
	421	C	LEU A	53	53.383	2.879	-4.975	1.00	52.64 58.35
	422 423	0 N	LEU A ASN A	53	52.319	2.688	-4.348	1.00	38.80
10	424	CA	ASN A	54 54	53.708 52.820	4.055 5.195	-5.500	1.00	47.61
	425	СВ	ASN A	54	53.638	6.453	-5.344 -5.089	1.00 1.00	60.77
	426	CG	ASN A	54	54.433	6.376	-3.804	1.00	62.70 72.45
	427 428	OD1 ND2	ASN A ASN A	54	53.865	6.317	-2.708	1.00	70.70
15	429	C	ASN A	54 54	55.761 51.905	6.373 5.420	-3.927	1.00	70.84
	430	0	ASN A	54	52. 30 8	5.246	-6.534 -7.678	1.00 1.00	55.42 52.22
	431	N	ILE A	55	50.669	5.807	-6.241	1.00	47.52
	432 433	CA CB	ILE A ILE A	5 5 5 5	49.681	6.089	-7.267	1.00	48.77
20	434	CG2	ILE A	55	48.459 47.338	5.177 5.670	-7.138 -8.055	1.00	48.20
	435	CG1	ILE A	55	48.848	3.746	-7.493	1.00 1.00	64.85 17.58
	436 437	CD1	ILE A	55	47.667	2.811	-7.511	1.00	22.96
	437 438	C	ILE A	55 55	49.242	7.528	-7.070	1.00	53.16
25	439	Ň	VAL A	56	48.602 49.576	7.862 8.374	-6.062 -8.041	1.00 1.00	50.16
	440	CA	VAL A	56	49.200	9.784	-7.939	1.00	53.12 55.98
	441 442	CB CG1	VAL A	56	50.475	10.660	-8.216	1.00	53.06
	443	CG2	VAL A VAL A	56 56	50.160 51.656	12.096 10.181	-7.893	1.00	67.53
30	444	C ·	VAL A	56	48.109	10.161	-7.396 -8.867	1.00 1.00	38.93
	445	0	VAL A	56	48.152	9.979	-10.075	1.00	54.49 42.98
	446 447	N CA	ASN A ASN A	57	47.094	10.850	-8.287	1.00	63.99
	448	CB	ASN A	57 57	45.941 46.339	11.323 12.495	-9.041 -9.945	1.00	72.29
35	449	CG	ASN A	57	46.916	13.667	-9.157	1.00 1.00	88.41 95.72
	450	OD1	ASN A	57	46.274	14.182	-8.236	1.00	90.65
	451 452	ND2 C	ASN A ASN A	57 57	48.133	14.089	-9.512	1.00	90.43
	453	ŏ	ASN A	57	45.413 45.349	10.169 10.232	-9.866 -11. 0 89	1.00 1.00	67.43
40	454	N _.	ALA A	58	45.046	9.107	-9.161	1.00	76.76 65.44
	455 456	CA CB	ALA A	58	44.526	7.893	-9.764	1.00	59.50
	457	C	ALA A ALA A	58 58	43.813 43.591	7.065 8.128	-8.715	1.00	51.61
	458	0	ALA A	58	42.696	8.976	-10.925 -10.860	1.00 1.00	56.95 59.56
45	459	N.	LYS A	59	43.815	7.356	-11.984	1.00	54.03
	460 461	CA CB	LYS A LYS A	59 50	42.999	7.392	-13.188	1.00	56.80
	462	CG	LYS A	59 59	43.897 44.932	7.371 8.485	-14.432 -14.454	1.00	52.13
~~	463	CD	LYS A	59	46.010	8.238	-14.454 -15.500	1.00 1.00	75.19 87.07
50	464	CE	LYS A	59	47.122	9.272	-15.379	1.00	101.21
	465 466	NZ C	LYS A LYS A	59	48.271	8.958	-16.271	1.00	106.25
	467	ŏ	LYS A	59 59	42.171 42.354	6.106 5.318	-13.095 -12.167	1.00	51.59
E E	468	N	PHE A	60	41.241	5.888	-14.015	1.00 1.00	37.92 54.25
55	469 470	CA	PHE A	60	40.470	4.657	-13.946	1.00	48.76
	470 471	CB CG	PHE A PHE A	60 60	39.250	4.729	-14.854	1.00	54.70
	472	CD1	PHE A	60	38.304 38.495	5.832 7.117	-14.506 -15.002	1.00 1.00	37.20
۲0	473	CD2	PHE A	60	37.215	5.583	-13.684	1.00	29.43 37.72
60	474 475	CE1	PHE A	60	37.606	8.134	-14.687	1.00	40.04
	476	CE2 CZ	PHE A PHE A	60 60	36.315 36.510	6.597	-13.358	1.00	23.38
	477	Č	PHE A	60	41.388	7.875 3.529	-13.860 -14.397	1.00 1.00	30.49 45.95
65	478	0	PHE A	60	41.263	2.389	-13.957	1.00	37.39
υJ	479 480	N CA	GLU A	61	42.326	3.865	-15.276	1.00	48.08
	481	CB	GLU A GLU A	61 61	43.279 44.195	2.887 3.535	-15.782	1.00	61.34
	482	CG	GLU A	61	43.508	3.525 3.900	-16.842 -18.170	1.00 1.00	72.31 91.97
70	483	CD	GLU A	61	42.606	5.127	-18.061	1.00	102.49
70	484	OE1	GLU A	61	43.123	6.227	-17.758	1.00	100.34

	485 486	OE2 C	GLU A	61 · 61	41.381 44.116	4.993 2.335	-18.283 -14.625	1.00 1.00	100.98 57.54
	487 488	0	GLU A	61	44.781	1.306	-14.754	1.00	53.72
5	489	N CA	ASP A ASP A	62 62	44.078	3.027	-13.493	1.00	48.67
-	490	CB	ASP A	62 62	44.837 45.141	2.597 3.784	-12.330	1.00	40.78
	491	CG	ASP A	62	46.284	4.654	-11.407 -11.920	1.00	58.38
	492	OD1	ASP A	62	47.343	4.090	-12.281	1.00 1.00	55.63
	493	OD2	ASP A	62	46.122	5.898	-11.947	1.00	50.67 65.51
10	494	Ç	ASP A	62	44.104	1.519	-11.547	1.00	32.95
	495	0	ASP A	62	44.699	0.839	-10.711	1.00	33.25
	496 497	N CA	SER A	63	42.808	1.374	-11.800	1.00	27.08
	498	CB	SER A SER A	63 63	42.038	0.346	-11.111	1.00	24.76
15	499	OG	SER A	63	40.574 39.976	0.381 1.632	-11.542 -11.254	1.00	32.81
	500	C	SER A	63	42.639	-1.002	-11.500	1.00 1.00	57.02 36.75
	501	0	SER A	63	43.468	-1.094	-12.419	1.00	30.75
	502	N	GLY A	64	42.236	-2.057	-10.809	1.00	34.81
20	503	CA	GLY A	64	42.790	-3.348	-11.160	1.00	42.02
20	504 505	C O	GLY A	64	43.349	-4.182	-10.021	1.00	50.47
	506	Ň	GLY A GLU A	64 65	43.011 44.224	-4.005 5.107	-8.ö50	1.00	48.47
	507	ČA	GLU A	65	44.836	-5.107 -6.021	-10.387 -9.436	1.00	51.85
	508	CB	GLU A	65	44.691	-7.448	·9.953	1.00 1.00	43.33
25	509	CG	GLU A	65	45.405	-8.502	9.135	1.00	52.77 52.38
	510	CD	GLU A	65	45.636	-9.792	-9.907	1.00	58.39
	511	OE1	GLU A	65	46.528	-9.798	-10.801	1.00	43.40
	512 513	OE2	GLU A	65	44.917	-10.782	-9.610	1.00	51.74
30	514	C	GLU A GLU A	65 65	46.309	-5.711	-9.240	1.00	45.24
50	515	Ň	TYR A	6 5 6 6	47.057 46.726	-5.550 -5.644	-10.212	1.00	39.10
	516	CA	TYR A	6 6	48.119	-5.363	-7.981 -7.664	1.00 1.00	40.60
	517	СВ	TYR A	66	48.259	-4.029	-6.936	1.00	35.48 18.93
25	518	CG	TYR A	66	48.056	-2.817	-7.810	1.00	24.42
35	519	CD1	TYR A	6 6	46.801	-2.218	·7.927	1.00	27.62
	520 521	CE1 CD2	TYR A	66	46.618	-1.068	-8.707	1.00	20.61
	522	CE2	TYR A TYR A	66 66	49.131	-2.240	-8.493	1.00	20.62
	523	CZ	TYR A	66	48.968 47.708	-1.093 -0.506	-9.268 -0.375	1.00	19.14
40	524	OH	TYR A	66	47.546	0.631	-9.375 -10.149	1.00 1.00	37.26 20.86
	525	С	TYR A	66	48.692	-6.454	-6.789	1.00	20.86 35.81
	526	0	TYR A	66	47.992	-6.973	-5.888	1.00	26.54
	527	N	LYS A	67	49.950	-6.803	-7.071	1.00	20.27
45	528 529	CA CB	LYS A Lys a	67 ~~	50.672	-7.827	-6.316	1.00	42.77
13	530	CG	LYS A Lys a	67 67	50 <i>.2</i> 77 50.131	-9.255 -9.502	-6.735	1.00	42.46
	531	CD	LYS A	67	49.867	-10.987	-8.223 -8.489	1.00 1.00	70.28
	532	CE	LYS A	67	49.313	-11.233	·9.888	1.00	66.50 73.20
50	533	NZ	LYS A	67	49.387	-12.668	-10.255	1.00	55.01
50	534	Ç	LYS A	67	52.161	-7.648	-6.480	1.00	49.35
	535 536	0	LYS A	67	52.656	-7.502	-7.596	1.00	49.27
	537	N CA	CYS A CYS A	68	52.872	-7.632	-5.359	1.00	55.09
	538	Č	CYS A	68 68	54.314 54.966	-7.450 -8.793	-5.384 5.474	1.00	54.74
55	539	ŏ	CYS A	68	54.285	-9.748	-5.171 -4.779	1.00 1.00	42.46
	540	СВ	CYS A	68	54.750	-6.451	-4.309	1.00	18.20 64.47
	541	SG	CYS A	68	54.393	-6.915	-2.586	1.00	100.38
	542	N	GLN A	69	56.267	-8.876	-5.444	1.00	26.58
60	543 544	CA	GLN A	69	56.968	-10.142	-5.299	1.00	26.57
00	545	CB CG	GLN A	69 60	56.693	-10.973	-6.556	1.00	15.18
	546	CD	GLN A GLN A	69 69	57.877 57.573	-11.704 -12.192	-7.156 -9.567	1.00	38.54
	547	OE1	GLN A	69	56.511	-12.192 -12.787	-8.567 -8.816	1.00 1.00	36.61
	548	NE2	GLN A	69	58.497	-11.941	-9.498	1.00	18.42 36.58
65	549	Ç	GLN A	69	58.472	-10.000	-5.034	1.00	41.83
	550	0	GLN A	69	59.174	-9.343	-5.804	1.00	24.51
	551 552	N CA	HIS A	70	58.951	-10.602	-3.938	1.00	59.31
	552 553	CA CB	HIS A	70 70	60.375	-10.552	-3.568	1.00	54.15
70	554	CG	HIS A HIS A	70 70	60.550 60.025	-10.461 -0.104	-2.050	1.00	49.67
			, 110 X	70	60.025	-9.194	-1.451	1.00	57.18

	555	CD2	HIS A	70-	59.202	-8.984	-0.397	1.00	57.85
	556	ND1	HIS A	70	60.376	-7.946	-1.918	1.00	60.44
	557 550	CE1	HIS A	70	59.796	-7.021	-1.178	1.00	62.11
5	558 559	NE2	HIS A	70	59.078	-7.624	-0.246	1.00	69.17
5	560	C	HIS A HIS A	70 70	61. 065 60.390	-11.814	-4.055	1.00	45.74
	561	Ň	GLN A	70 71	62.397	-12.760 -11.824	-4.466 4.000	1.00	48.46
	562	CA	GLN A	71	63.170	-12.998	-4.020 -4.434	1.00	34.41
	563	CB	GLN A	71	64.631	-12.609	4.631	1.00 1.00	34.74
10	564	CG	GLN A	71	65.521	-13.746	-5.061	1.00	28.64 28.58
	565	CD	GLN A	71	67.021	-13.427	-4.933	1.00	44.36
	566	OE1	GLN A	71	67.508	-12.432	-5.447	1.00	24.64
	567	NE2	GLN A	71	67.749	-14.289	-4.246	1.00	82.76
15	568	C	GLN A	71	63.098	-14.123	-3.76	1.00	42.41
13	569 570	0 N	GLN A GLN A	71	63.036	-13.876	-2.168	1.00	58.78
	571	CA	GLN A	72 72	63.116 63.062	-15.369	-3.622	1.00	36.65
	572	CB	GLN A	72 72	64.225	-16.493 -16.440	-2.873 -1.894	1.00	56.26
	573	čĠ	GLN A	72	65.522	-16.962	-1.694 -2.419	1.00 1.00	66.55
20	574	CD	GLN A	72	66.614	-10.771	-1.409	1.00	74.96 81.18
	575	OE1	GLN A	72	66.932	-15.625	-1.027	1.00	46.66
	576	NE2	GLN A	72	67.196	-17.886	-0.944	1.00	86.79
	577	Ç	GLN A	72	61.791	-16.614	-2.044	1.00	47.57
25	578	0	GLN A	72	61.763	-17.006	-1.035	1.00	53.55
25	579	N	VAL A	73	60.740	-15.937	-2.457	1.00	25.14
	580	CA CB	VAL A	73	59.499	-16.027	-1.737	1.00	27.76
	581 582	CB CG1	VAL A VAL A	73 70	59.434	-14.865	-0.770	1.00	24.20
	583	CG2	VAL A VAL A	73 73	58.034 60.349	-14.638 -15.143	-0.284	1.00	61.77
30	584	Č	VAL A	73	58.330	-16.018	0.383 -2.730	1.00 1.00	48.95
	585	ō	VAL A	73	58.405	-15.385	-3.793	1.00	38.97 50.48
	586	N	ASN A	74	57.261	-16.735	-2.392	1.00	30.12
	587	CA	ASN A	74	56.080	-16.794	-3.251	1.00	54.75
25	588	CB	ASN A	74	55.023	-17.677	-2.576	1.00	65.77
35	589	CG	ASN A	74	55.444	-19.138	-2.523	1.00	77.30
•	590	OD1	ASN A	74	55.408	-19.840	-3.538	1.00	66.94
	591 592	ND2	ASN A ASN A	74	55.871	-19.586	-1.341	1.00	98.68
	593	CO	ASN A	74 74	55.514 55.945	-15.392 -14.384	-3.593	1.00	61.15
40	594	Ň	GLU A	7 5	54.553	-15.322	-3.027 -4.523	1.00	65.55
. •	595	CA	GLU A	75	53.971	-14.057	-4.951	1.00 1.00	62.19 63.45
	596	CB	GLU A	75	53.296	-14.213	-6.314	1.00	82.08
	597	CG	GLU A	75	54.237	-14.649	-7.425	1.00	101.46
40	598	CD	GLU A	75	53.533	-14.804	-8.759	1.00	105.08
45	599	OE1	GLU A	75	52.308	-14.564	-8.815	1.00	85.23
	600	OE2	GLU A	75	54.204	-15.167	-9.747	1.00	113.01
	601	C	GLU A	7 5	52.979	-13.531	-3.920	1.00	46.81
	602 603	0 N	GLU A SER A	75 76	52.180	-14.279	-3.376	1.00	63.28
50	604	CA	SER A	76 76	53.008 52.104	-12.216 -11.602	-3.667 -2.698	1.00	44.23
	605	CB	SER A	76	52.265	-10.080	-2.698	1.00 1.00	44.01
	606	OG	SER A	76	51.674	-9.502	-3.854	1.00	52.11 49.14
	607	С	SER A	76	50.658	-11.942	-3.036	1.00	40.30
	608	0	SER A	76	50.351	-12.409	-4.122	1.00	37.45
55	609	N	GLU A	77	49.787	-11.733	-2.074	1.00	47.16
	610	CA	GLU A	77	48.373	-11.965	-2.345	1.00	50.65
	611	CB	GLU A	<u>77</u>	47.596	-12.125	-1.037	1.00	64.23
	612 613	CO CD	GLU A GLU A	77	48.051	-13.299	-0.184	1.00	100.08
60	614	OE1	GLU A	77 77	49.143	-12.917	0.795	1.00	121.85
•	615	OE2	GLU A	77	49.535 49.607	-11.731 -13.804	0.817 1. 54 3	1.00	113.34
	616	c c	GLU A	77	47.780	-10.837	-3.181	1.00 1.00	135.86 57.00
	617	ŏ	GLU A	77	48.203	-9.696	-2.996	1.00	70.10
	618	N	PRO A	78	46.905	-11.147	-4.089	1.00	60.36
65	619	CD	PRO A	78	48.349	-12.453	-4.468	1.00	76.75
	620	CA	PRO A	78	46.348	-10.084	-4.915	1.00	45.94
	621	CB	PRO A	78	45.380	-10.826	-5.830	1.00	63.85
	622 623	ÇG	PRO A	78	45.954	-12.210	-5.903	1.00	74.36
70	624	CO	PRO A PRO A	78 79	45.640 45.047	-9.054 0.220	-4.055	1.00	46.99
	~~	•	FRU A	78	45.047	-9.380	-3.014	1.00	44.78

	625	N	VAL A	79 -	45.723	-7.806	-4.493	1.00	20 76
	626	CA	VAL A	79	45.068	-6.708	-3.808	1.00	38.75 46.98
	627	CB:	VAL A	79	46.101	-5.836	-3.067	1.00	48.31
5	628	CG1	VAL A	79	45.700	-4.371	-3.099	1.00	58.66
J	629 630	CG2	VAL A	79	46.195	-6.289	-1.639	1.00	43.93
	631	C	VAL A VAL A	79 70	44.344	-5.925	-4.907	1.00	41.63
	632	N	VAL A TYR A	79 80	44.974	-5.465 5.700	-5.869	1.00	31.43
	633	ČA	TYR A	80	43.024 42.258	-5. 799 -5.105	-4.786	1.00	36.26
10	634	CB	TYR A	80	40.986	-5.105 -5.889	·5.807	1.00	43.25
	635	CG	TYR A	80	41.315	-7.289	-6.142 -6.619	1.00 1.00	43.58
	636	CD1	TYR A	80	41.297	-8.370	·5.734	1.00	62.18 59.18
	637	CE1	TYR A	80	41.695	-9.639	-6.138	1.00	63.70
	638	CD2	TYR A	80	41.738	-7.521	-7.932	1.00	64.60
15	639	CE2	TYR A	80	42.141	-8.793	-8.341	1.00	72.36
	640	CZ	TYR A	80	42.116	-9.843	-7.439	1.00	71.99
	641	он	TYR A	80	42.511	-11.0 96	-7.848	1.00	86.14
	642 643	C	TYR A	80	41.920	-3.677	-5. 468	1.00	39.91
20	644	ίχi	TYR A LEU A	80	41.299	-3.392	-4.445	1.00	39.73
20	645	CA	LEU A	81 81	42.350 42.130	-2.791	-6.356	1.00	42.49
	646	CB	LEU A	81	43.462	-1.367 -0.645	-6.23 6	1.00	39.83
	647	ĊĠ	LEU A	81	43.433	0.870	-6.434 -6.520	1.00	29.82
	648	CD1	LEU A	81	42.862	1.449	-5.246	1.00 1.00	35.37
25	649	CD2	LEU A	81	44.841	1.363	-6.750	1.00	54.76 51.99
	650	С	LEU A	81	41.113	-0.953	-7.307	1.00	40.44
	651	0	LEU A	81	41.218	-1.335	-8.479	1.00	44.23
	652	N	GLU A	82	40.119	-0.175	-6.903	1.00	34.19
30	653	CA	GLU A	82	39.108	0.266	-7.850	1.00	43.16
20	654 655	CB CG	GLU A	82	37.833	-0.540	-7.615	1.00	43.29
	656	CD	GLU A GLU A	82	36.683	-0.166	-8.517	1.00	64.74
	657	OE1	GLU A	82 82	35.546	-1.157	-8.415	1.00	79.52
	658	OE2	GLU A	82	35.177 35.023	-1.505 -1.586	-7.272	1.00	89.05
35	659	Č	GLU A	82	38.802	1.778	-9.468 -7.803	1.00	95.85
	660	Ö	GLU A	82	38.213	2.268	-6.840	1.00 1.00	36.44 20.88
	661	N	VAL A	83	39.200	2.505	-8.849	1.00	20.88 17.32
	662	CA	VAL A	83	38.957	3.947	-8.947	1.00	20.25
40	663	CB	VAL A	83	39.842	4.587	-10.012	1.00	16.19
40	664	CG1	VAL A	83	39.647	6.071	-9. 99 5	1.00	22.13
	665 666	CG2	VAL A	83	41.280	4.219	-9.786	1.00	30.28
	667	C	VAL A VAL A	83	37.503	4.274	-9.323	1.00	24.88
	668	Ñ	PHE A	83 84	36.946	3.744	-10.285	1.00	47.06
45	669	CA CA	PHE A	84	36.894 35.520	5.162 5.575	-8.555	1.00	14.13
	670	CB	PHE A	84	34.646	5.374	-8.800 -7.564	1.00 1.00	26.86
	671	CG	PHE A	84	34.475	3.964	-7.1 63	1.00	13.44
	672	CD1	PHE A	84	35.571	3.183	-6.840	1.00	34.33 45.55
~~	673	CD2	PHE A	84	33.205	3.420	-7.070	1.00	44.61
50	674	CE1	PHE A	84	35.405	1.865	-6.433	1.00	65.24
	675	CE2	PHE A	84	33.022	2.106	-6.667	1.00	42.90
	676 677	cz	PHE A	84	34.122	1.325	-6.343	1.00	65.66
	677 678	Ö	PHE A	84	35.462	7.061	-9.146	1.00	45.25
55	679	Ñ	SER A	84 85	36.490	7.760	- 9. i 78	1.00	38.34
-	680	CA	SER .	85 85	34.234 33.919	7.512	-6.3 99	1.00	46.62
	681	CB	SER A	8 5	34.232	8.899 9.236	-9.712	1.00	37.65
	682	ÖĞ	SER A	85	34.067	10.629	-11.159 -11.358	1.00	40.40
	683	С	SER A	85	32.438	9.035	-9.467	1.00 1.00	35.89 22.78
60	684	0	SER A	85	31.630	8.613	-10.264	1.00	37.65
	685	N	ASP A	86	32.098	9.604	-8.326	1.00	14.50
	686	CA	ASP A	86	30.713	9.771	-7.919	1.00	9.43
	687	CB	ASP A	86	30.133	8.405	-7.554	1.00	12.45
65	688 689	CG	ASP A	86	28.611	8.418	-7.427	1.00	51.60
5 5	690	OD1 OD2	ASP A	86 86	28.054	9.224	-6.645	1.00	55.89
	691	C	ASP A ASP A	86 86	27.960	7.606	-8.115	1.00	79.60
	692	ŏ	ASP A ASP A	86 86	30.746 31 B27	10.707	-6.680	1.00	28.99
	693	Ň	TRP A	87	31.827 29.583	11.076 11.104	-6.199	1.00	31.21
70	694	CA	TRP A	87	29.543	11.104	-6.171 -5.024	1.00	14.11
			• • • • •		-0.070		-5.024	1.00	41.60

	695 696 697	CD2 CB		A 87 A 87 A 87	28.161 27.790 28.221	12.643 13.509 14.858	-4.893 -6.057 -6.312	1.00 1.00 1.00	67.93 79.67
5	698 699	CE2 CE3	TRP A	A 87 A 87	27.641 29.040	15.256 15.762	-7.532	1.00	97.15 98.87
	700 701	CD1 NE1	TRP	A 87	26.995	13.162	-5.626 -7.102	1.00 1.00	106.42 73.69
	702	CZ2	TRP /	A 87	26.898 27.851	14.205 16.513	-7.994 -8.083	1.00 1.00	66.94 111.64
10	703 704	CZ3 CH2	TRP /	A 87 A 87	29.246 28.654	17.010 17.375	-6.174 -7.392	1.00 1.00	116.11
	705 706	C	TRP /		29.900 30.629	11.273 11.811	-3.735	1.00	119.60 44.35
	707	N	LEU /	A 88	29.368	10.071	-2.915 -3.546	1.00 1.00	41.60 50.46
15	708 709	CA CB	LEU /		29.659 28.394	9.311 9.038	-2.340 -1.530	1.00 1.00	36.94 4.59
	710 711	CG CD1	LEU /		27.705 26.690	10.219 9.649	-0.861	1.00	21.69
	712 713	CD2	LEU /	A 88	28.720	11.117	0.161 -0.155	1.00 1.00	11.07 21.48
20	714	C O	LEU /	A 88	30.289 29.805	7.981 7.248	-2.655 -3.508	1.00 1.00	28.38 29.21
	715 716	N CA	LEU /		31.370 32.077	7.676 6.409	-1.948 -2.092	1.00	45.92
	717 718	CB CG	LEU /	A 89	33.474	6.637	-2.623	1.00 1.00	35.41 12.22
25	719	CD1	LEU /		34.333 33.477	5.406 4.296	-2.839 -3.405	1.00 1.00	32.05 25.06
	720 721	CD2 C	LEU A		35.530 32.153	5.774 5.786	-3.801 -0.721	1.00 1.00	25.39
	722 723	O N	LEU A	A 89	32.513	6.454	0.234	1.00	21.36 48.70
30	724	CA	LEU A	A 90	31.757 31.798	4.528 3.848	-0.602 0.690	1.00 1.00	31.16 20.27
	725 726	CB CG	LEU A		30.677 30.650	2.856 2.184	0.796 2.145	1.00 1.00	4.59
	727 728	CD1 CD2	LEU A	A 90	30.229	3.221	3.170	1.00	5.03 5.42
35	729	C	LEU A	4 90	29.601 33.099	1.067 3.096	2.147 0.757	1.00 1.00	18.53 29.48
	730 731	O N	GLN A		33.291 34.004	2.129 3.557	0.017 1.612	1.00 1.00	49.50 33.11
	732 733	CA CB	GLN A	91	35.308 36.389	2.930	1.724	1.00	34.25
40	734	ca	GLN A	91	36.487	4.007 4.900	1.872 0.664	1.00 1.00	29.25 4.72
	735 736	CD OE1	GLN A		37.564 37.492	5.950 6.821	0.795 1.657	1.00 1.00	24.07 33.85
	737 738	NE2 C	GLN A		38.566 35.339	5.885	-0.075	1.00	25.90
45	739	0	GLN A	91	34.607	1.961 2.134	2.892 3.875	1.00 1.00	39.46 41.60
•	740 741	N CA	ALA A		36.162 36.256	0.922 -0.064	2.774 3.844	1.00 1.00	33.12 44.90
	742 743	CB C	ALA A		35.425 37.696	-1.288 -0.476	3.498	1.00	44.46
50	744	0	ALA A	92	38.544	-0.586	4.151 3.253	1.00 1.00	45.76 51.50
	745 746	N CA	SER A	93	37.962 39.286	-0.702 -1.103	5.432 5.881	1.00 1.00	48.03 52.40
	747 748	CB OG	SER A		39.265 38.305	-1.381 -2.377	7.380	1.00	48.05
55	749	C	SER A	93	39.671	-2.364	7.689 5.142	1.00 1.00	47.42 49.91
	750 751	O N	SER A		40.837 38.659	-2.593 -3.170	4.836 4.856	1.00 1.00	54.70 47.64
	752 753	CA CB	ALA A		38.830 39.567	-4.430 -5.404	4.161	1.00	40.55
60	754	C	ALA A	94	37.441	-4.968	5.048 3.823	1.00 1.00	44.76 53.40
	755 756	O N	ALA A		36.554 37.249	-5.033 -5.347	4.688 2.565	1.00 1.00	40.13 63.75
	757 758	CA CB	GLU A		35.964 35.952	-5.865 -5.940	2.125	1.00	61.37
65	759 760	CG	GLU. A	95	36.118	-4.576	0.603 -0.059	1.00 1.00	77.66 76.66
	761	CD OE1	GLU A	95	36.098 36.111	-4.640 -3.565	-1.582 -2.217	1.00 1.00	96.68 107.34
	762 763	OE2 C	GLU A		36.073 35.680	-5.754 -7.231	-2.151	1.00	100.79
70	764	Ŏ	GLU A		34.527	-7.667	2.750 2.838	1.00 1.00	54.28 42.98

	765 766	N CA	VAL A VAL A	96 96	36.739 36.604	-7.903 -9.205	3.193 3.851	1.00 1.00	61.87 61.01
•	767 768	CB: CG1	VAL A	96	36.933	-10.354	2.897	1.00	56.77
5	769	CG2	VAL A VAL A	96	36.541	-11.670	3.536	1.00	39.60
,	770	C	VAL A VAL A	96 96	36.215	-10.149	1.576	1.00	53.03
	771	ŏ	VAL A	96	37.520 38.751	-9.306 0.302	5.084	1.00	56.97
	772	Ň	VAL A	97	36.900	-9.202 -9.512	4.985	1.00	45.37
	773	CA	VAL A	97	37.614	-9.606	6.241 7.499	1.00	53.01
10	774	СВ	VAL A	97	37.188	-8.448	8.435	1.00 1.00	56.01
	775	CG1	VAL A	97	37.790	-8.628	9.802	1.00	57.61 87.18
	776	CG2	VAL A	97	37.637	-7.122	7.858	1.00	68.07
	777	C	VAL A	97	37.372	-10.944	8.209	1.00	61.52
15	778	0	VAL A	97	36.278	-11.542	8.158	1.00	38.67
13	779 780	N	MET A	98	38.412	-11.411	8.879	1.00	64.69
	780 781	CA CB	MET A	98	38.335	-12.644	9.633	1.00	62.72
	782	CG	MET A MET A	98	39.745	-13.081	10.013	1.00	71.28
	783	SD	MET A	98 98	39.901 39.346	-14.561	10.252	1.00	94.38
20	784	CE	MET A	98	37.821	-15.500 -16.041	8.803	1.00	75.29
	785	C	MET A	98	37.520	-12.336	9.448 10.894	1.00	93.84
	786	0	MET A	98	37.748	-11.318	11.552	1.00 1.00	58.92 61.33
	7 87	N	GLU A	99	36.573	-13.201	11.241	1.00	61.37
05	788	CA	GLU A	99	35.762	-12.971	12.436	1.00	59.89
25	789	CB	GLU A	99	34.950	-14.211	12.797	1.00	52.02
	790	CG	GLU A	99	0153	-14.039	14.072	1.00	64.75
	791 700	CD	GLU A	99	33.366	-15. 28 5	14.456	1.00	90.18
	792 793	OE1 OE2	GLU A	99	33.983	-16.375	14.536	1.00	106.04
30	793 794	C	GLU A GLU A	99	32.137	-15.170	14.685	1.00	84.66
50	795	ŏ	GLU A	99 99	36.621 37.583	-12.587	13.633	1.00	66.15
	796	Ň	GLY A	100	36.265	-13.284 -11.478	13.972	1.00	81.55
	797	CA	GLY A	100	37.016	-11.021	14 <i>.</i> 271 15.419	1.00	58.33
	798	C	GLY A	100	37.943	-9.872	15.088	1.00 1.00	54.87 54.97
35	799	0	GLY A	100	38.293	-9.087	15.960	1.00	69.91
	800	N	GLN A	101	38.367	-9.772	13.836	1.00	54.17
	801	CA	GLN A	101	39.237	-8.671	13.445	1.00	57.48
	802	CB	GLN A	101	39.942	-8.998	12.125	1.00	60.93
40	803 804	CG CD	GLN A	101	41.016	-10.063	12.237	1.00	76.51
TV	805	OE1	GLN A GLN A	101	42.059	-9.719	13.290	1.00	90.62
	806	NE2	GLN A	101 101	41.825 43.212	-9.891 - 9.85	14.490	1.00	100.86
	807	C	GLN A	101	38.445	-9.215 -7.353	12.846 13.311	1.00	85.92
	808	ŏ	GLN A	101	37.210	-7.333 -7.337	13.344	1.00 1.00	56.15
45	809	N	PRO A	102	39.151	-6.222	13.180	1.00	44.69
	810	CD	PFO A	102	40.600	-5.991	13.326	1.00	56.36 60.77
	811	CA	PRO A	102	38.438	-4.954	13.048	1.00	55.67
	812	CB	PRO A	102	39.483	-3.933	13.458	1.00	47.18
50	813	ÇG	PRO A	102	40.742	-4.538	12.918	1.00	47.65
50	814 815	C	PRO A	102	37.915	-4.716	11.631	1.00	58.48
	816	O N	PRO A	102	38.567	-5.036	10.635	1.00	58.71
	817	CA CA	LEU A LEU A	103 103	36.719	-4.151	11.569	1.00	1.34ن
	818	CB	LEU A	103	36.041 34.728	-3.833	10.320	1.00	47.87
55	819	ČĞ	LEU A	103	33.811	-4.610 -4.304	10.248 9.073	1.00	54.63
	820	CD1	LEU A	103	34.546	-4.59 6	7.767	1.00 1.00	54.99
	821	CD2	LEU A	103	32.537	-5.130	9.206	1.00	57.13 49.78
	822	C	LEU A	103	35.761	-2.332	10.359	1.00	39.79
60	823	0	LEU A	103	35.046	-1.847	11.254	1.00	21.76
60	824	N	PHE A	104	36.300	-1.598	9.391	1.00	18.87
	825	CA	PHE A	104	36.111	-0.157	9.393	1.00	30.54
	826	CB	PHE A	104	37.466	0.500	9.616	1.00	41.57
	827 828	CG CD1	PHE A	104	37.385	1.948	9.969	1.00	54.55
65	829	CD1	PHE A PHE A	104	37.282	2.351	11.301	1.00	72.72
	830	CE1	PHE A	104 104	37.441	2.917	8.975	1.00	57.49
	831	CE2	PHE A	104	37.227 37.385	3.706 4.273	11.640	1.00	70.88
	832	CZ	PHE A	104	37.285	4.273 4.670	9.297 10.633	1.00	60.17
	833	C	PHE A	104	35.466	0.437	8.137	1.00 1.00	66.74 35.62
70	834	0	PHE A	104	36.079	0.468	7.066	1.00	37.03
*					-				۵،.۵

	835	N	LEU A	105	34.234	0.922	8.269	1.00	
	836	CA	LEU A	105	33.541	1.550	7.144	1.00 1.00	36.14
	837	CB	LEU A	105	32.073	1.154	7.125	1.00	48.60 46.94
5	838 839	CG.	LEU A	105	31.870	-0.297	6.725	1.00	52.90
J	840	CD1 CD2	LEU A LEU A	105	30.385	-0.564	6.516	1.00	46.80
	841	C	LEU A LEU A	105	32.663	-0.562	5.442	1.00	53.92
	842	ŏ	LEU A	105 105	33.658 33.938	3.072	7.195	1.00	46.53
	843	N	ARG A	106	33.406	3.645 3.725	8.241 6.066	1.00	50.68
10	844	CA	ARG A	106	33.539	5.172	6.066 5.962	1.00 1.00	45.66
	845	CB	ARG A	106	35.021	5.513	5.786	1.00	26.49
	846	CG	ARG A	106	35.354	6.951	5.450	1.00	36.08 14.61
	847	CD	ARG A	106	36.798	7.050	4.915	1.00	5.55
15	848 849	NE	ARG A	106	37.271	8.435	4.831	1.00	20.40
13	850	CZ NH1	ARG A ARG A	106	38.344	8.828	4.148	1.00	31.42
	851	NH2	ARG A	106 106	39.064	7.946	3.479	1.00	46.98
	852	C	ARG A	106	38.700 32.770	10.107 5.674	4.129	1.00	48.19
	853	ō	ARG A	106	32.812	5.073	4.756 3.681	1.00	33.55
20	854	N	CYS A	107	32.077	6.789	4.929	1.00 1.00	52.61
	855	CA	CYS A	107	31.320	7.373	3.829	1.00	27.72 41.84
	856	Ç	CYS A	107	32.088	8.567	3.283	1.00	22.10
	857	0	CYS A	107	31.791	9.699	3.617	1.00	21.70
25	858 859	CB	CYS A	107	29.941	7.816	4.309	1.00	53.08
23	860	SG N	CYS A	107	28.736	8.075	2.959	1.00	81.46
	861	CA	HIS A HIS A	108	33.097	8.301	2.461	1.00	28.20
	862	CB	HIS A	108 108	33.951 35.203	9.338	1.869	1.00	34.09
	863	ČĞ	HIS A	108	35.203 36.204	8.680 9.643	1.301	1.00	40.04
30	864	CD2	HIS A	108	36.947	9.629	0.762	1.00	35.83
	865	ND1	HIS A	108	36.593	10.766	-0.371 1.460	1.00 1.00	36.86
	866	CE1	HIS A	108	37.536	11.397	0.779	1.00	36.99 45.07
	867	NE2	HIS A	108	37.767	10.725	-0.334	1.00	23.01
35	868	C	HIS A	108	33.251	10.165	0.774	1.00	42.71
<i>JJ</i>	869 870	0	HIS A	108	32.719	9.638	-0.199	1.00	37.25
	871	N CA	GLY A GLY A	109	33.269	11.480	0.946	1.00	49.87
	872	Č	GLY A GLY A	109 109	32.623	12.365	-0.006	1.00	29.45
	873	ŏ	GLY A	109	33.537 34.721	12.894	-1.088	1.00	26.33
40	874	Ň	TRP A	110	32.939	13.111 13.111	-0.879 -2.263	1.00	19.36
	875	CA	TRP A	110	33.697	13.598	-2.263 -3.404	1.00 1.00	35.74
	876	CB	TRP A	110	32.731	13.903	-4.564	1.00	32.65 20.29
	877	CG	TRP A	110	33.447	14.390	-5.792	1.00	22.58
45	878 879	CD2	TRP A	110	34.199	13.610	-6.731	1.00	26.60
73	880	CE2 CE3	TRP A TRP A	110	34.759	14.506	-7.667	1.00	16.42
	881	CD1	TRP A TRP A	110 110	34.452	12.242	-6.864	1.00	20.97
	882	NE1	TRP A	110	33.584 34.350	15.673	-6.187	1.00	16.06
	883	CZ2	TRP A	110	35.572	15.760 14.088	-7.312 -8.734	1.00	29.92
50	884	CZ3	TRP A	110	نة.260	11.817	-7.931	1.00 1.00	11.79
	885	CH2	TRP A	110	35.812	12.748	-8.853	1.00	46.44 19.66
	886	Ç	TRP A	110	34.565	14.791	-3.047	1.00	29.32
	887	0	TRP A	110	34.162	15.708	-2.335	1.00	21.14
55	888 889	N CA	ARG A	111	35.814	14.736	-3.559	1.00	32.25
J J	890	CB	ARG A ARG A	111	36.819	15.806	-3.372	1.00	51.05
	891	ČĠ	ARG A	111 111	36. 29 4 36. 33 5	17.122	-3.911	1.00	55.38
	892	CD	ARG A	111	37.728	17.249 16.914	-5.405	1.00	82.45
	893	NE	ARG A	111	37.701	16.807	-5.919 -7.377	1.00	117.48
60	894	cz	ARG A	111	38.779	16.716	-8.149	1.00 1.00	137.24 143.04
	895	NH1	ARG A	111	39.988	16.721	-7.60 1	1.00	142.25
	896	NH2	ARG A	111	38.650	16.625	-9.468	1.00	146.91
	897 800	Ç	ARG A	111	37.110	16.070	-1.919	1.00	61.58
65	898 899	O	ARG A	111	37.239	17.225	-1.504	1.00	77.35
-	800	N CA	asn a Asn a	112	37.217	15.017	-1.101	1.00	59.89
	901	CB	ASN A	112 112	37.433	15.116	0.363	1.00	47.67
	902	ČĞ	ASN A	112	38.892 39.700	15.480 14.277	0.648	1.00	68.19
	903	OD1	ASN A	112	39.474	13.725	1.106 2.188	1.00	77.01
70	904	ND2	ASN A	112	40.669	13.866	2.188 0.282	1.00 1.00	77.39
							V.aiUE	1.00	78.90

	905 906 907	C O	ASN A ASN A	112 112	36.433 36.705	16.068 16.745	0.984 1.990	1.00 1.00	28.46 47.00
	908	N CA	TRP A	113 113	35.263	16.090	0.367	1.00	35.39
5	909	CB	TRP A	113	34.201 33.208	16.977 17.136	0.819	1.00	51.08
	910	CG	TRP A	113	32.539	18.373	-0.253 0.147	1.00 1.00	64.97
	911	CD2	TRP A	113	32.917	19.678	-0.301	1.00	81.55 74.85
	912	CE2	TRP A	113	32.014	20.570	0.303	1.00	85.26
10	913 914	CE3 CD1	TRP A TRP A	113	33.902	20.163	-1.1 7 7	1.00	61.05
	915	NE1	TRP A TRP A	113 113	31.496 31.158	18.519	0.997	1.00	83.43
	916	CZ2	TRP A	113	32.073	19.856 21.949	1.104 0.055	1.00	83.67
	917	CZ3	TRP A	113	33.958	21.536	-1.420	1.00 1.00	96.42
15	918	CH2	TRP A	113	33.046	22.396	-0.803	1.00	72.53 92.25
13	919 920	CO	TRP A	113	33.482	16.590	2.066	1.00	46.75
	921	N	TRP A ASP A	113 114	33.409 32.921	15.393	2.379	1.00	35.50
	922	CA	ASP A	114	32.243	17.551 17.1 7 3	2.792	1.00	63.72
20	923	CB	ASP A	114	32.177	18.380	4.025 4.943	1.00 1.00	64.61
20	924	CG	ASP A	114	33.506	18.737	5.602	1.00	86.45 98.41
	925	OD1	ASP A	114	34.402	17.872	5.707	1.00	84.34
	926 927	OD2 C	ASP A ASP A	114	33.641	19.918	6.023	1.00	109.32
	928	ŏ	ASP A	114 114	30.871 30.070	16.558 17.044	3.829	1.00	61.40
25	929	Ñ	VAL A	115	30.569	15.463	3.039 4.556	1.00	81.69
	930	CA	VAL A	115	29.265	14.772	4.391	1.00 1.00	39.40 37.88
	931	CB	VAL A	115	29.491	13.274	4.126	1.00	10.52
	932 933	CG1 CG2	VAL A	115	28.209	12.621	3.617	1.00	5.47
30	934	C	VAL A VAL A	115 115	30.635 28.364	13.071	3.147	1.00	9.13
	935	ŏ	VAL A	115	28.807	14.928 14.733	5.596 6.740	1.00	28.56
	936	N	TYR A	116	27.101	15.273	5.384	1.00 1.00	19.72 37.21
	937	CA	TYR A	116	26.192	15.428	6.517	1.00	46.14
35	938 939	CB CG	TYR A	116	25.652	16.857	6.574	1.00	61.34
	940	CD1	TYR A TYR A	116 116	26.725 27.203	17.921 18.582	6.689	1.00	76.00
	941	CE1	TYR A	116	28.190	19.572	5.557 5.658	1.00 1.00	87.94
	942	CD2	TYR A	116	27.264	18.269	7.931	1.00	91.76 84.35
40	943 944	CE2 CZ	TYR A	116	28.255	19.255	8.041	1.00	88.13
	945	OH	TYR A TYR A	116 116	28.709 29.683	19.897	6.899	1.00	83.79
	946	Č.	TYR A	116	25.022	20.859 14.449	6. 98 8 6.489	1.00 1.00	79.96
	947	0	TYR A	116	24.764	13.805	5.461	1.00	48.03 47.24
45	948 949	N	LYS A	117	24.313	14.360	7.618	1.00	49.04
73	950	CA CB	LYS A Lys a	117	23.175	13.455	7.754	1.00	62.64
	951	čĠ	LYS A	117 117	21.940 21.382	14.043 15.296	7.066	1.00	84.33
	952	CD	LYS A	117	20.779	15.016	7.713 9.087	1.00 1.00	103.44
50	953	CE	LYS A	117	20.018	16.235	9.606	1.00	122.93 125.37
J U	954 955	NZ C	LYS A	117	19.408	16.006	10.942	1.00	122.53
	956	ŏ	LYS A Lys a	117 117	23.543	12.117	7.115	1.00	59.71
	957	Ň	VAL A	118	22.858 24.636	11.626 11.532	6.207 7.588	1.00	73.62
EE	958	ÇA	VAL A	118	25.107	10.262	7.057	1.00 1.00	36.40 27. 9 2
55	959	CB	VAL A	118	26.612	10.090	7.262	1.00	4.59
	960 961	CG1 CG2	VAL A	118	27.021	8.714	6.845	1.00	4.58
	962	C	VAL A VAL A	118 118	27.369 24.421	11.124	6.440	1.00	27.69
	963	ŏ	VAL A	118	24.371	9.071 8.943	7.685 8.897	1.00 1.00	21.65
60	964	N	ILE A	119	23.882	8.205	6.843	1.00	23.38 29.44
	965 966	CA	ILE A	119	23.222	7.008	7.313	1.00	32.32
	967	CB CG2	ILE A ILE A	119	21.749	7.038	7.026	1.00	15.68
	968	CG1	ILE A ILE A	119 119	21.120 21.116	5.711	7.453	1.00	9.94
65	969	CD1	ILE A	119	19.568	8.205 8.203	7.779 7.722	1.00	16.41
	970	C	ILE A	119	23.817	5.818	6.605	1.00 1.00	28.41 41.89
	971 972	O N	ILE A	119	24.159	5.901	5.424	1.00	51.23
	973	CA	TYR A TYR A	120 120	23.973	4.719	7.330	1.00	34.78
70	974	CB	TYR A	120	24.530 25.732	3.531 3.013	6.720 7.510	1.00	31.98
			• •			5.015	7.510	1.00	6.64

	975 976	CG CD1	TYR A TYR A	120 120	26.965 27.192	3.845 4.931	7.362	1.00	4.59
	977	CE1	TYR A	120	28.354	5.687	8.175 8.055	1.00	7.90
_	978	CD2	TYR A	120	27.912	3.527	6.413	1.00 1.00	5.34
5	979	CE2	TYR A	120	29.085	4.271	6.270	1.00	8.49 23.20
	980	CZ	TYR A	120	29.304	5.353	7.090	1.00	24.78
	981	ОН	TYR A	120	30.467	6.077	6.927	1.00	41.99
	982 983	C	TYR A	120	23.454	2.476	6.672	1.00	39.78
10	984	0 N	TYR A TYR A	120	22.664	2.339	7.614	1.00	25.06
10	985	CA	TYR A TYR A	121 121	23.406 22.421	1.748	5.564	1.00	40.70
	986	CB	TYR A	121	21.497	0.694 0.982	5.421	1.00	43.93
	987	ca	TYR A	121	20.739	2.288	4.248 4.367	1.00	37.43
	988	CD1	TYR A	121	21.387	3.511	4.161	1.00 1.00	49.95
15	989	CE1	TYR A	121	20.691	4.723	4.262	1.00	49.22 56.51
	99C	CD2	TYR A	121	19.369	2.303	4.678	1.00	25.20
	991	CE2	TYR A	121	18.664	3.494	4.783	1.00	32.17
	992	CZ	TYR A	121	19.326	4.709	4.572	1.00	58.52
20	993 994	ОН	TYR A	121	18.632	5.904	4.685	1.00	47.56
20	995	C O	TYR A	121	23.095	-0.65u	5.206	1.00	57.82
	996	Ñ	TYR A LYS A	121 122	23.997	-0.778	4.341	1.00	56.35
	997	CA	LYS A	122	22.677 23.216	-1.636 -2.978	6.003	1.00	50.06
	998	СВ	LYS A	122	23.790	-3.497	5.881 7.209	1.00	54.50
25	999	CG	LYS A	122	24.742	-4.667	7.027	1.00 1.00	66.15
	1000	CD	LYS A	122	24.992	-5.443	8.315	1.00	79.15 81.56
	1001	CE	LYS A	122	23.821	-6.355	8.653	1.00	78.05
	1002	NZ	LYS A	122	24.119	-7.213	9.829	1.00	89.70
20	1003	Č	LYS A	122	22.040	-3.841	5.463	1.00	56.73
30	1004	0	LYS A	122	21.202	-4.210	6.289	1.00	47.59
	1005 1006	N CA	ASP A	123	21.978	-4.138	4.168	1.00	66.50
	1007	CA CB	ASP A ASP A	123	20.911	-4.951	3.599	1.00	73.31
	1008	CG	ASP A	123 123	20.768 21.977	-6.270 -7.186	4.365	1.00	80.64
35	1009	OD1	ASP A	123	22.334	-7.186 -7.499	4.190 3.031	1.00 1.00	94.21
	1010	OD2	ASP A	123	22.568	-7.600	5.214	1.00	103.57
	1011	С	ASP A	123	19.591	-4.203	3.608	1.00	97.62 74.17
	1012	0	ASP A	123	18.616	-4.644	4.220	1.00	66.73
40	1013	N.	GLY A	124	19.571	-3.062	2.928	1.00	75.26
40	1014	CA	GLY A	124	18.362	-2.265	2.851	1.00	79.44
	1015 1016	CO	GLY A	124	17.954	-1.637	4.166	1.00	80.57
	1017	N	GLY A GLU A	124 125	17.323 18.301	-0.580 -2.2 9 5	4.186	1.00	91.15
	1018	CA	GLU A	125	17.981	-2.2 85 -1.786	5.268 6.594	1.00	74.63
45	1019	CB	GLU A	125	18.066	-2.914	7.616	1.00 1.00	61.74
	1020	CG	GLU A	125	17.092	-4.054	7.365	1.00	79.17 98.38
	1021	CD	GLU A	125	15.642	-3.619	7.478	1.00	106.78
	1022	OE1	GLU A	125	15.235	-3.167	8.570	1.00	118.36
50	1023	OE2	GLU A	125	14.907	-3.728	6.475	1.00	110.58
20	1024 1025	C	GLU A	125	18.947	-0.660	6.981	1.00	58.10
	1025	N	GLU A ALA A	125	20.161	-0.697	6.664	1.00	30.38
	1027	ČA	ALA A	126 126	18.399 19.185	0.343 1.490	7.662	1.00	50.55
	1028	CB	ALA A	126	18.322	2.732	8.088 8.098	1.00	52.07
55	1029	C	ALA A	126	19.795	1.272	9.461	1.00 1.00	53.61 45.73
	1030	0	ALA A	126	19.077	1.194	10.459	1.00	48.02
	1031	N .	LEU A	127	21.122	1.179	9.491	1.00	34.72
	1032	CA	LEU A	127	21.895	0.979	10.720	1.00	30.29
60	1033	CB	LEU A	127	23.358	0.751	10.350	1.00	15.93
00	1034 1035	CG CD1	LEU A LEU A	127	23.473	-0.487	9.465	1.00	4.91
	1036	CD2	LEU A	127 127	24.904 22.935	-0.710	9.010	1.00	4.59
	1037	C	LEU A	127	21.782	-1.692 2.175	10.260	1.00	16.61
	1038	ŏ	LEU A	127	22.724	2.175 2.962	11.660	1.00	21.97
65	1039	Ň.	LYS A	128	20.635	2.305	11.801 12.315	1.00 1.00	23.95 19.75
	1040	CA	LYS A	128	20.391	3.427	13.205	1.00	29.37
	1041	СВ	LYS A	128	19.091	3.206	13.951	1.00	16.78
	1042	CG	LYS A	128	17.911	2.993	13.019	1.00	47.56
70	1043	CD	LYS A	128	16.603	2.817	13.777	1.00	56.74
70	1044	CE	LYS A	128	15.492	2.380	12.824	1.00	58. 6 8

	1045 1046 1047	NZ C O	LYS A LYS A LYS A	128 128 128	14.183 21.529 22.289	2.220 3.647	13.519 14.187	1.00	55.73 40.15
	1048	Ň	TYR A	129	21.647	4.599 2.757	14.064	1.00	53.09
5	1049	ĊA	TYR A	129	22.707	2.757	15.1 59 16.144	1.00	36.41
	1050	СВ	TYR A	129	23.134	1.465	16.629	1.00 1.00	37.61
	1051	CG	TYR A	129	22.011	0.668	17.256	1.00	55.67 69.76
	1052	CD1	TYR A	129	21.225	-0.184	16.491	1.00	84.41
10	1053	CE1	TYR A	129	20.152	-0.868	17.051	1.00	80.71
10	1054	CD2	TYR A	129	21.699	0.813	18.604	1.00	78.34
	1055 1056	CE2 CZ	TYR A TYR A	129	20.632	0.136	19.172	1.00	85.65
	1057	OH	TYR A	129 129	19.860 18.794	-0.702 -1.369	18.391	1.00	81.90
	1058	Č	TYR A	129	23.938	3.635	18.952	1.00	78.93
15	1059	ō	TYR A	129	24.414	4.513	15.664 16.379	1.00 1.00	41.39
	1060	N	TRP A	130	24.451	3.321	14.475	1.00	73.88 21.26
	1061	CA	TRP A	130	25.630	4.021	13.983	1.00	55.41
	1062	CB	TRP A	130	26.227	3.270	12.798	1.00	66.63
20	1063	CG	TRP A	130	26.560	1.867	13.090	1.00	78.03
20	1064	CD2	TRP A	130	27.747	1.387	13.717	1.00	80.17
	1065 1066	CE2 CE3	TRP A	130	27.652	-0.021	13.762	1.00	96.27
	1067	CD1	TRP A	130 130	28.889	2.009	14.244	1.00	63.46
	1068	NE1	TRP A	130	25.807	0.770	12.791	1.00	95.81
25	1069	CZ2	TRP A	130	26.456 28.657	-0.371 -0.822	13.189	1.00	93.15
	1070	CZ3	TRP A	130	29.888	1.215	14.314 14.7 9 2	1.00	106.12
	1071	CH2	TRP A	130	29.764	-0.188	14.823	1.00 1.00	70.51 97.78
	1072	С	TRP A	130	25.397	5.477	13.569	1.00	69.95
20	1073	0	TRP A	130	26.292	6.113	13.027	1.00	86.40
30	1074	N	TYR A	131	24.215	6.013	13.841	1.00	75.40
	1075	CA	TYR A	131	23.916	7.387	13.449	1.00	97.14
	1076 1077	CB	TYR A	131	22.479	7.739	13.825	1.00	111.94
	1077	CG CD1	TYR A TYR A	131	21.976	8.995	13.151	1.00	148.46
35	1079	CE1	TYR A	131 131	21.452 20.988	8.958	11.863	1.00	154.63
	1080	CD2	TYR A	131	22.025	10.111 10.223	11.242 13.800	1.00	166.01
	1081	CE2	TYR A	131	21.566	11.383	13.187	1.00 1.00	162.09 169.95
	1082	CZ	TYR A	131	21.046	11.320	11.909	1.00	172.27
40	1083	ОН	TYR A	131	20.578	12.465	11.306	1.00	171.20
40	1084	C	TYR A	131	24.854	8.424	14.048	1.00	107.44
	1085	0	TYR A	131	25.432	9.238	13.326	1.00	112.84
	1086	N	GLU A	132	24.991	8.410	15.368	1.00	111.22
	1087 1088	CA CB	GLU A GLU A	132	25.857	9.362	16.047	1.00	114.10
45	1089	CG	GLU A	132 132	26.071 24.802	8.954	17.505	1.00	121.12
	1090	CD	GLU A	132	25.067	8.888 8.459	18.342 19.774	1.00	146.81
	1091	OE1	GLU A	132	26.243	8.195	20.104	1.00 1.00	156.70 168.06
	1092	OE2	GLU A	132	24.100	8.386	20.565	1.00	164.60
	1093	С	GLU A	132	27.212	9.442	15.359	1.00	112.41
50	1094	0	GLU A	132	27.715	10.523	15.090	1.00	126.08
	1095	N	ASN A	133	27.792	8.286	15.065	1.00	107.15
•	1096	CA	ASN A	133	29.101	8.246	14.436	1.00	110.99
	1097 1098	CB CG	ASN A	133	29.828	6.972	14.874	1.00	132.56
55	16:19	OD1	asn a Asn a	133 133	29.903 30.195	6.843	16.381	1.00	152.00
	1100	ND2	ASN A	133	29.636	7.810 5.653	17.084	1.00	156.21
	1101	C	ASN A	133	29.071	8.366	16.882 12.913	1.00 1.00	164.20 103.70
	1102	0	ASN A	133	28.344	7.653	12.236	1.00	103.53
60	1103	N	HIS A	134	29.885	9.274	12.388	1.00	108.74
60	1104	CA	HIS A	134	29.987	9.520	10.954	1.00	130.31
	1105	CB	HIS A	134	30.880	10.729	10.703	1.00	148.82
	1106	CG	HIS A	134	30.457	11.949	11.454	1.00	166.98
	1107	CD2	HIS A	134	31.030	12.601	12,493	1.00	171.29
65	1108 1109	ND1 CE1	HIS A HIS A	134	29.283	12.620	11.183	1.00	179.56
	1110	NE2	HIS A HIS A	134 134	29.153 30.196	13.629	12.026	1.00	185.16
	1111	C	HIS A	134	30.186	13.641 8.320	12.829 10.242	1.00	183.14
	1112	ō	HIS A	134	30.194	8.013	9.120	1.00 1.00	130.17 144.97
 -	1113	N	ASN A	135	31.506	7.668	10.891	1.00	115.50
70	1114	CA	ASN A	135	32.133	6.470	10.351	1.00	106.66
								-	

	1115 1116	CB CG	ASN A ASN A	135 135	33.641 34.357	6.677 6.732	10.201	1.00	111.41
	1117	OD1	ASN A	135	33.734	6.607	11.535 12.590	1.00 1.00	121.66 137.22
_	1118	ND2	ASN A	135	35.671	6.919	11.493	1.00	131.58
5	1119	С	ASN A	135	31.848	5.256	11.226	1.00	98.67
	1120	0	ASN A	135	31.560	5.429	12.414	1.00	95.00
	1121 1122	N CA	ILE A	136	31.914	4.084	10.657	1.00	84.56
	1123	CB	ILE A	136 136	31.590 30.615	2.901 2.005	11.441 10.689	1.00	68.70
10	1124	CG2	ILE A	136	30.242	0.824	11.556	1.00 1.00	70.57 57.24
	1125	CG1	ILE A	136	29.371	2.809	10.308	1.00	76.41
	1126	CD1	ILE A	136	28.315	1.994	9.607	1.00	81.35
	1127	C	ILE A	136	32.825	2.108	11.771	1.00	67.79
15	1128 1129	0 N	ILE A SER A	136 137	33.484 33.153	1.575 2.051	10.879	1.00	75.89
13	1130	CA	SER A	137	34.327	1.314	13.057 13.512	1.00 1.00	64.01
	1131	CB	SER A	137	35.240	2.228	14.319	1.00	50.08 42.18
	1132	OG	SER A	137	36.435	1.547	14.654	1.00	74.65
20	1133	C	SER A	137	33.882	0.137	14.366	1.00	40.13
20	1134	0	SER A	137	33.257	0.331	15.402	1.00	31.91
	1135 1136	N CA	ILE A	138	34.172	-1.079	13.915	1.00	47.57
	1137	CB	ILE A	138 138	33.767 32.849	-2.272 -3.173	14.646 13.801	1.00 1.00	55.59
	1138	CG2	ILE A	138	32.360	-4.317	14.646	1.00	45.34 52.83
25	1139	CG1	ILE A	138	31.640	-2.378	13.310	1.00	55.63
	1140	CD1	ILE A	138	30.680	-3.166	12.457	1.00	59.56
	1141	Ç	ILE A	138	35.014	-3.039	15.023	1.00	69.36
	1142	0	ILE A	138	35.542	-3.824	14.243	1.00	86.80
30	1143 1144	N CA	THR A	139 139	35.481 36.687	-2.793 2.412	16.238	1.00	80.29
50	1145		THRA	139	36.824	-3.412 -3.094	16.765 18.243	1.00 1.00	71.05
	1146	OG1	THR A	139	35.584	-3.396	18.894	1.00	65.21 63.19
	1147	CG2	THR A	139	37.152	-1.610	18.429	1.00	37.67
25	1148	Ç	THR A	139	36.727	-4.906	16.577	1.00	73.17
35	1149	o S	THR A	139	37.633	-5.439	15.927	1.00	72.09
	1150 1151	N CA	ASN A	140	35.731	-5.585 7.004	17.126	1.00	71.99
	1152	CB	ASN A	140 140	35.689 35.704	-7.021 -7.615	17.012 18.427	1.00 1.00	74.50
	1153	ČĠ	ASN A	140	37.023	-8. 292	18.747	1.00	83.94 102.78
40	1154	OD1	ASN A	140	37.329	-9.296	18.114	1.00	129.44
	1155	ND2	ASN A	140	37.842	-7.797	19.666	1.00	102.21
	1156	C	ASN A	140	34.509	-7.489	16.134	1.00	66.79
	1157 1158	0 N	ASN A ALA A	140	33.351	-7.495 7.974	16.568	1.00	67.94
45	1159	CA	ALA A	141 141	34.834 33.851	-7.874 -8.305	14.888 13.887	1.00 1.00	51.28
	1160	CB	ALA A	141	34.536	-8.441	12.546	1.00	50.10 44.66
	1161	С	ALA A	141	33.037	-9.568	14.167	1.00	57.39
	1162	0	ALA A	141	_ 33.395	-10.379	15.013	1.00	76.44
50	1163	N OA	THR A		~ 31.940	-9.721	13.424	1.00	63.44
J U	1164 1165	CA CB	THR A	142	31.029 29.830	-10.864	13.548	1.00	68.80
	1166	OG1	THR A	142 142	30.292	-10.522 -9.914	14.429 15.637	1.00	56.28
	1167	CG2	THR A	142	29.038	-11.771	14.756	1.00 1.00	69.20 63.60
	1168	С	THR A	142	30.476	-11.284	12.186	1.00	63.69 77.84
55	1169	0	THR A	142	30.350	-10.467	11.275	1.00	84.69
	1170	N	VAL A	143	30.133	-12.562	12.053	1.00	80.43
	1171 1172	CA CB	VAL A	143	29.594	-13.071	10.800	1.00	75.62
	1173	CG1	VAL A	143 143	29.347 28.297	-14.600 -14.907	10.870	1.00	62.57
60	1174	CG2	VAL A	143	28.903	-15.123	11.934 9.516	1.00 1.00	69.07 78.52
	1175	C	VAL A	143	28.282	-12.361	10.472	1.00	73.71
	1176	0	VAL A	143	27.893	-12.285	9.307	1.00	85.08
	1177	N	GLU A	144	27.593	-11.846	11.491	1.00	65.50
65	1178	CA CB	GLU A	144	26.347	-11.130	11.245	1.00	78.86
UJ	1179 1180	CB CG	GLU A	144	25.554	-10.974	12.544	1.00	88.26
	1181	CD	GLU A	144 144	24.140 23.389	-10.450 -10.299	12.348 13.656	1.00	123.20
	1182	OE1	GLU A	144	23.977	-10.29 8 -10.598	13.656 14.717	1.00 1.00	142.61 141.13
~~	1183	OE2	GLU A	144	22.212	-9.883	13.620	1.00	155.89
70	1184	С	GLU A	144	26.611	-9.767	10.616	1.00	84.50

	1185	0	GLU A	144	25.793	-9.241	9.855	1.00	86.40
	1186	N	ASP A	145	27.764	-9.198	10.943	1.00	83.52
	1187	CA	ASP A	145	28.139	-7.913	10.383	1.00	73.54
5	1.188 1189	CB CG	ASP A ASP A	145	29.429	-7.402	11.033	1.00	81.77
•	1190	OD1	ASP A	145 145	29.191 28.336	-6.826 5.014	12.430	1.00	98.36
	1191	OD2	ASP A	145	29.856	-5.914 -7.280	12.559 13.394	1.00	102.22
	1192	C	ASP A	145	28.317	-8.028	8.875	1.00 1.00	95.71
	,1193	0	ASP A	145	28.626	-7.053	8.211	1.00	65.16 74.60
10	1194	N	SER A	146	28.112	-9.224	8.337	1.00	63.10
	1195	CA	SER A	146	28.246	-9.460	6.906	1.00	51.02
	1196	CB	SER A	146	28.403	-10.959	6.619	1.00	62.55
	1197 1198	OG	SER A	146	29.671	-11.452	7.030	1.00	53.04
15	1199	C	SER A SER A	146	26.997	-8. 94 9	6.221	1.00	50.62
13	1200	Ň	GLY A	146 147	25. 93 5 27.130	-8.865	6.848	1.00	44.95
	1201	ČA	GLY A	147	25.992	-8.609 -8.119	4.942 4.185	1.00	48.93
	1202	Č	GLY A	147	26.389	-7.039	3.199	1.00 1.00	55.32 60.64
	1203	0	GLY A	147	27.587	-6.725	3.051	1.00	55.89
20	1204	Ŋ	THR A	148	25.396	-6.477	2.510	1.00	61.14
	1205	CA	THR A	148	25.665	-5.415	1.540	1.00	66.29
	1206 1207	CB OG1	THR A	148	24.735	-5.502	0.318	1.00	67.47
	1207	CG2	THR A THR A	148	23.514	-4.813	0.604	1.00	89.27
25	1209	C	THR A	148 148	24.414 25.442	-6.954 4.064	-0.006	1.00	53.85
	1210	ŏ	THR A	148	24. 37 3	-4.064 -3.805	2.229 2.793	1.00	60.43
	1211	Ň	TYR A	149	26.461	-3.214	2.783	1.00 1.00	48.98
	1212	CA	TYR A	149	26.371	-1.911	2.836	1.00	56.49 46.76
20	1213	CB	TYR A	149	27.600	-1.648	3.726	1.00	50.51
30	1214	CG	TYR A	149	27.679	-2.436	5.010	1.00	37.62
	1215 1216	CD1 CE1	TYR A	149	28.197	-3.727	5.030	1.00	38.64
	1217	CD2	TYR A TYR A	149	28.288	-4.446	6.214	1.00	21.54
	1218	CE2	TYR A	149 149	27.252 27.336	-1.882 -2.589	6.211	1.00	27.02
35	1219	cz	TYR A	149	27.854	-2.569 -3.868	7.393 7.390	1.00 1.00	25.84
	1220	ОН	TYR A	149	27.923	-4.562	8.573	1.00	22.38 47.89
	1221	Ç	TYR A	149	26.329	-0.824	1.775	1.00	47.29
	1222	0	TYR A	149	26. 62 6	-1.059	0.590	1.00	37.99
40	1223 1224	N CA	TYR A	150	25.962	0.369	2.225	1.00	35.54
40	1225	CB	TYR A TYR A	150 150	25.947	1.547	1.380	1.00	37.17
	1226	ČĠ	TYR A	150	25.029 23.546	1.341 1.438	0.165 0.440	1.00	20.88
	1227	CD1	TYR A	150	22.897	2.667	0.465	1.00 1.00	11.30
4.5	1228	CE1	TYR A	150	21.518	2.751	0.712	1.00	12.45 32.37
45	1229	CD2	TYR A	150	22.789	0.299	0.668	1.00	24.35
	1230	CE2	TYR A	150	21.412	0.374	0.909	1.00	20.64
	1231 1232	CZ OH	TYR A	150	20.784	1.599	0.933	1.00	30.87
	1233	C	TYR A TYR A	150 150	19.428	1.673	1.174	1.00	44.40
50	1234	ŏ	TYR A	150	25.492 24.661	2.711 2.544	2.250 3.170	1.00	39.54
	1235	Ň	CYS A	151	26.062	3.882	1.987	1.00 1.00	10.94
	1236	CA	CYS A	151	25.705	5.052	2.757	1.00	36.69 45.12
	1237	Ç	CYS A	151	25.007	6.072	1.908	1.00	51.21
55	1238	0_	CYS A	151	25.146	6.112	0.686	1.00	60.75
23	1239 1240	CB	CYS A	151	26.931	5.677	3.410	1.00	44.14
	1240	SG N	CYS A	151	28.208	6.239	2.230	1.00	79.82
	1242	ČA	THR A THR A	152 152	24.258	6.891	2.606	1.00	48.42
	1243	CB	THR A	152	23.500 22.068	7.959 7.517	1.949 1.650	1.00	39.06
60	1244	OG1	THR A	152	21.399	8.531	0.891	1.00 1.00	43.65 41.96
	1245	CG2	THR A	152	21.310	7.257	2.942	1.00	52.65
	1246	C	THR A	152	23.555	9.204	2.825	1.00	38.12
	1247	0	THR A	152	23.025	9.224	3.943	1.00	25,44
65	1248	N	GLY A	153	24.215	10.236	2.307	1.00	56.51
05	1249 1250	CA C	GLY A	153	24.377	11.477	3.048	1.00	57.72
	1251	ŏ	GLY A GLY A	153 153	24.335	12.680	2.112	1.00	54.16
	1252	Ň	LYS A	154	24.362 24.309	12.540 13.842	0.903	1.00	50.60
	1253	CA	LYS A	154	24.227	14.969	2.706 1.840	1.00 1.00	38.84 51.33
70	1254	CB	LYS A	154	23.115	15.878	2.356	1.00	63.30

	1255	CG	LYS A	154	23,445	17.360	2.388	1.00	70.00
	1256	CD							72.63
			LYS A	154	22.595	18.054	3.439	1.00	102.12
	1257	CE	LYS A	154	23.004	19.508	3.589	1.00	114.39
	1258	NZ .	LYS A	154	22.404	20.128			
5							4. 7 97	1.00	116.75
3	1259	С	LYS A	154	25.591	15.650	1.647	1.00	43.23
	1260	0	LYS A	154	26.393	15.769	2.565	1.00	
	1261	Ñ							25.84
				155	25.799	16.110	0.410	1.00	50.07
	1262	CA	VAL A	155	27.053	16.754	0.017	1.00	48.54
	1263	СВ	VAL A	155	27.920	15.801			40.54
10							-0.810	1.00	44.27
10	1264	CG1	VAL A	155	29.142	16.517	-1.363	1.00	33.53
	1265	CG2	VAL A	155	28.341	14.619	0.032		55.55
								1.00	57.29
	1266	С	VAL A	155	26.752	18.008	-0.791	1.00	67.17
	1267	0	VAL A	155	26.127	17.926	-1.839	1.00	75.50
	1268	N	TRP A	156	27.200				
15						19.158	-0.290	1.00	71.27
15	1269	CA	TRP A	156	26.950	20.433	-0.941	1.00	74.25
	1270	СВ	TRP A	156	27.792	20.531	-2.227	1.00	
									82.77
	1271	CG	TRP A	156	27.663	21.880	-2.856	1.00	95.08
	1272	CD2	TRP A	156	27.991	23.118	-2.237	1.00	99.06
	1273	CE2	TRP A	156	27.707				
20						24.146	-3 .172	1.00	109.06
20	1274	CE3	TRP A	156	28.499	23.466	-0.981	1.00	92.83
	1275	CD1	TRP A	156	27.202	22.187	-4.115	1.00	
	1276								103.95
		NE1	TRP A	156	27.22 6	23.548	-4.308	1.00	101.14
	1277	CZ2	TRP A	156	27.915	25.505	-2.883	1.00	117.16
	1278	CZ3	TRP A						
25				156	28.708	24.820	-0.691	1.00	111.82
25	1279	CH2	TRP A	156	28.415	25.823	-1.644	1.00	117.54
	1280	С	TRP A	156	25.451	20.622	-1.252		
								1.00	77.62
	1281	0	TRP A	156	25.074	20.840	-2.391	1.00	86.35
	1282	N	GLN A	157	24.612	20.526	-0.216	1.00	
	1283	CA	GLN A						65.28
20				157	23.148	20.731	-0.292	1.00	81.65
30	1284	CB	GLN A	157	22.904	22.189	-0.665	1.00	97.92
	1285	CG	GLN A	157	23.502	23.199			
							0.312	1.00	117.66
	1286	CD	GLN A	157	23.208	24.631	-0.086	1.00	136.93
	1287	OE1	GLN A	157	22.533	24.882	-1.084	1.00	146.04
	1288	NE2	GLN A						
25				157	23.616	25.725	0.549	1.00	141.98
35	1289	C	GLN A	157	22.274	19. 79 0	-1.165	1.00	79.89
	1290	0	GLN A	157	21.156	20.148	-1.533		
								1.00	84.84
	1291	N	LEU A	158	22,779	18.632	-1.485	1.00	73.68
	1292	CA	LEU A	158	22.000	17.633	-2.253	1.00	79.20
	1293	CB	LEU A	158	22.364				
40						17.659	-3.749	1.00	79.50
40	1294	CG	LEU A	158	22.096	18.967	-4.507	1.00	86.09
	1295	CD1	LEU A	158	22.474	18.815	-5.972	1.00	
	1296	CD2							76.62
			LEU A	158	20.647	19.379	-4.373	1.00	92.41
	1297	С	LEU A	158	22.262	16.262	-1.673	1.00	70.21
	1298	0	LEU A	158	23.390				
45						15.914	-1.325	1.00	65.09
43	1299	N	ASP A	159	21.236	15.470	-1.538	1.00	60.67
	1300	CA	ASP A	159	21.404	14.148	-0.999	1.00	
	1301	CB							55.55
			ASP A	159	20.088	13.617	-0.446	1.00	67.04
	1302	CG	ASP A	159	19.493	14.534	0.596	1.00	100.18
	1303	OD1	ASP A	159	20.141				
50						14.767	1.640	1.00	107.25
JU	1304	OD2	ASP A	159	18.375	15.034	0.368	1.00	120.77
	1305	С	ASP A	159	21.937	13.199	-2.057	1.00	
	1306	ō							59.79
			ASP A	159	21.662	13.379	-3.258	1.00	71.48
	1307	N	TYR A	160	22.692	12.198	-1.619	1.00	40.00
	1308	CA	TYR A	160	23.237		-2.545		46.99
55			700			11.218		1.00	36.10
JJ	1309	CB	TYR A	160	24.620	11.639	-3.026	1.00	27.20
	1310	CG	TYR A	160	24.661	13.032	-3.599	1.00	
	1311	CD1	TVD A						48.59
			TYR A	160	24.780	14.143	-2.770	1.00	67.84
	1312	CE1	TYR A	160	24.805	15. 440	-3.297	1.00	85.53
	1313	CD2	TYR A	160					
60					24.570	13.246	-4.970	1.00	46.32
UU	1314	CE2	TYR A	160	24.592	14.538	-5.507	1.00	59.84
	1315	CZ	TYR A	160	24.713	15.630	-4.665	1.00	
	1316	ОH							78.07
			TYR A	160	24.740	16.912	-5.178	1.00	80.23
	1317	С	TYR A	160	23.314	9.852	-1.881	1.00	41.50
	1318	Ō	TYR A						
65				160	23.085	9.729	-0.67 5	1.00	33.36
Ų,	1319	N	GLU A	161	23.623	8.830	-2.675	1.00	46.21
	1320	CA	GLU A	161	23.725	7.469			
	1321						-2.173	1.00	42.10
		CB	GLU A	161	22.425	6.733	-2.462	1.00	40.63
	1322	CG	GLU A	161	22.451	5.247	-2.195	1.00	72.70
	1323	CD	GLU A						
70		_		161	21.042	4.640	-2.132	1.00	87.13
<i>1</i> U	1324	OE1	GLU A	161	20.932	3.391	-2.193	1.00	96.87
						= -			30.07

	1325	OE2	GLU A	161	20.049	5.405	-2.006	1.00	69.68
	1326 1327	C O ·	GLU A GLU A	161	24.898	6.793	-2.864	1.00	48.06
	1328	Ŋ	SER A	161 162	25.040 25.750	6.878 6.146	-4.080 -2.079	1.00	53.65
5	1329	CA	SER A	162	26.933	5.475	-2.079 -2.612	1.00 1.00	55.15
	1330	СВ	SER A	162	27.968	5.246	-1.498	1.00	57.03 68.17
	1331	Ó.	SER A	162	27.499	4.339	-0.501	1.00	46.93
	1332	Ç	SER A	162	26.572	4.138	-3.230	1.00	58.42
10	1333	0	SER A	162	25.476	3.615	-3.020	1.00	48.37
10	1334 1335	N CA	GLU A GLU A	163 163	27.498	3.587	-4.002	1.00	65.57
	1336	CB	GLU A	163	27.268 28.356	2.290 1.990	-4.619 -5.650	1.00	70.23
	1337	ČĞ	GLU A	163	28.293	2.834	-6.909	1.00 1.00	87.77 102.75
	7338	CD	GLU A	163	27.121	2.453	-7.797	1.00	103.75 115.27
15	1 339	OE1	GLU A	163	27.060	1.281	-8.229	1.00	111.84
	1340	OE2	GLU A	163	26.262	3.323	-8.062	1.00	129.74
	1341 1342	C	GLU A	163	27.366	1.282	-3.491	1.00	70.72
	1343	0 N	GLU A PRO A	163 164	28.244 26.460	1.387 0.300	-2.645	1.00	89.57
20	1344	CD	PRO A	164	25.401	-037	-3.448 -4.397	1.00 1.00	55.48
	1345	CA	PRO A	164	26.538	-0.684	-2.369	1.00	62.15 41.51
	1346	СВ	PRO A	164	25.363	-1.606	-2.663	1.00	42.71
	1347	ÇG	PRO A	164	25.250	-1.532	-4.128	1.00	64.09
25	1348	C	PRO A	164	27.877	-1.409	-2.399	1.00	38.62
23	1349 1350	0 N	PRO A LEU A	164	28.585	-1.386	-3.426	1.00	31.41
	1351	ČA	LEU A	165 165	28.234 29.498	-2.022 -2.753	-1.268 -1.151	1.00	33.57
	1352	CB	LEU A	165	30.540	-1.879	-0.490	1.00 1.00	25.38 26.45
	1353	CG	LEU A	165	31.924	-2.483	-0.322	1.00	25.16
30	1354	CD1	LEU A	165	32.619	-2.579	-1.655	1.00	29.84
	1355	CD2	LEU A	165	32.736	-1.587	0.602	1.00	42.13
	1356 1357	C	LEU A LEU A	165	29.278	-3.983	-0.306	1.00	26.10
	1358	Ň	ASN A	165 166	28.794 29.618	-3.876 -5.152	0.815 -0.838	1.00	33.23
35	1359	CA	ASN A	166	29.400	-6.398	-0.106	1.00 1.00	40.53 50.87
	1360	CB	ASN A	166	29.257	-7.59 5	-1.049	1.00	69.69
	1361	CG	ASN A	166	27.875	-7.698	-1.649	1.00	86.10
	1362	OD1	ASN A	166	26.895	-7.260	-1.034	1.00	58.55
40	1363 1364	ND2 C	ASN A ASN A	166 166	27.799	-8.292	-2.839	1.00	110.79
10	1365	ŏ	ASN A	166	30.537 31.703	-6.664 -6.667	0. 83 3 0.416	1.00 1.00	48.09
	1366	Ň	ILE A	167	30.193	-6.908	2.094	1.00	40.29 46.84
	1367	CA	ILE A	167	31,191	-7.165	3.119	1.00	53.30
45	1368	CB	ILE A	167	31.192	-6.039	4.156	1.00	54.88
45	1369	CG2	ILE A	167	31.949	-6.458	5.383	1.00	47.53
	1370 1371	CG1 CD1	ILE A ILE A	167	31.816	-4.791	3.545	1.00	48.70
	1372	C	ILE A	167 167	31.781 30.945	-3.603 -8.492	4.447 3.815	1.00	54.75
	1373	ŏ	ILE A	167	29.862	-8.731	4.388	1.00 1.00	59.98 39.94
50	1374	N	THR A	168	31.957	-9.353	3.777	1.00	61.65
	1375	CA	THR A	168	31.835	-10.666	4.386	1.00	68.33
	1376	CB	THR A	168	32.052	-11.774	3.343	1.00	80.46
	1377	OG1 CG2	THR A	168	31.627	-11.306	2.058	1.00	92.03
55	1379	C	THR A THR A	168 168	31.239 32.829	-13.010 -10.891	3.704	1.00	94.56
	1380	ŏ	THR A	168	34.031	-10.870	5.515 5.346	1.00 1.00	60.61
	1381	Ň	VAL A	169	32.313	-11.331	6.660	1.00	54.25 57.24
	1382	CA	VAL A	169	33.143	-11.638	7.820	1.00	64.14
60	1383	CB	VAL A	169	32.567	-11.028	9.083	1.00	54.63
UU	1384 1385	CG1	VAL A	169	33.436	-11.381	10.261	1.00	75.25
	1386	CG2 C	VAL A VAL A	169 169	32.470	-9.533	8.929	1.00	61.93
	1387	ŏ	VAL A VAL A	169	33.112 32.044	-13.156 -13.739	7.950 8.173	1.00	73.51
	1388	Ň	ILE A	170	34.268	-13.801	7.815	1.00 1.00	77.56 75.88
65	1389	CA	ILE A	170	34.312	-15.259	7.873	1.00	80.16
	1390	СВ	ILE A	170	35.341	-15.815	6.866	1.00	75.70
	1391	CG2	ILE A	170	34.778	-15.807	5.465	1.00	70.82
	1392 1393	CG1 CD1	ILE A	170	36.633	-15.007	6.932	1.00	90.89
70	1394	C	ILE A ILE A	170 170	37.719 34.568	-15.518 -15.970	6.004	1.00	107.17
, 🕶		_	164 A	.70	J-1,300	-15.879	9.246	1.00	87.00

	1395 1396	0	ILE A	170	35.373	-15.415	10.042	1.00	96.41
	1397	ČA	LYS A	171 171	33.843 34.002	-16.956 -17.747	9.475	1.00	84.91
	1398	CB	LYS A	171	32.777	-18.646	10.684 10.912	1.00 1.00	77.44
5	1399	CG	LYS A	171	32.895	-19.571	12.108	1.00	69.57 99.45
	1400	CD	LYS A	171	32.836	-18.812	13.422	1.00	104.18
	1401 1402	CE	LYS A	171	32.865	-19.773	14.611	1.00	104.74
	1402	NZ C	LYS A	171 171	32.737 35.260	-19.061 -18.572	15.914	1.00	93.90
10	1404	ŏ	LYS A	171	35.628	-18.860	10.523 9.376	1.00 1.00	84.98 94.71
	1405	N	ALA A	172	35.970	-19.012	11.575	1.00	87.21
	1406	CA	ALA A	172	37.223	-19.690	11.278	1.00	95.69
	1407 1408	CB C	ALA A	172	38.361	-18.758	11.670	1.00	93.23
15	1409	ŏ	ALA A	172 172	37.489 37.954	-21.071 -21.216	11.877 13.004	1.00	105.19
	1410	Ň	PRO A	173	37.149	-22.090	11.058	1.00 1.00	112.63 110.62
	1411	CD	PRO A	173	35.763	-22.015	10.625	1.00	99.89
	1412	CA	PRO A	173	37.466	-23.510	11.384	1.00	115.87
20	1413	CB	PRO A	173	36.690	-24.249	10.308	1.00	108.18
20	1414 1415	CG C	PRO A	173 173	35.438 38.974	-23.407 -23.790	10.162	1.00	104.37
	1416	ŏ	PRO A	173	39.763	-23.790 -23.104	11.504 10.878	1.00 1.00	128.43
	1417	Ň	ARG A	174	39.371	-24.790	12.289	1.00	141.54 133.44
0.5	1418	CA	ARG A	174	40.784	-25.147	12.416	1.00	142.76
25	1419	CB	ARG A	174	41.404	-24.373	13.578	1.00	151.84
	1420 1421	CG CD	ARG A	174	40.646	-24.535	14.896	1.00	162.79
	1422	NE	ARG A	174 174	40.099 38.922	-23.221 -23.410	15.420 16.282	1.00 1.00	169.70
	1423	CZ	ARG A	174	38.907	-23.284	17.609	1.00	176.81 177.27
30	1424	NH1	ARG A	174	40.007	-22.942	18.271	1.00	174.36
	1425	NH2	ARG A	174	37.770	-23.499	18.277	1.00	178.48
	1426 1427	C O	ARG A	174	40.973	-26.657	12.620	1.00	148.93
	1428	C1	ARG A	174 221	40.343 48.150	<i>-2</i> 7.476 13.699	11.946	1.00	150.68
35	1429	C2	NAG A	221	47.709	15.109	-5.031 -4.571	1.00 1.00	63.44 53.07
	1430	N2	NAG A	221	46.282	15.294	-4.715	1.00	54.52
	1431	C7	NAG A	221	45.470	14.819	-3.771	1.00	67.27
	1432 1433	O7 C8	NAG A	221	45.884	14.210	-2.774	1.00	51.25
40	1434	C3	NAG A NAG A	221 221	43.972 48.484	15.033 16.177	-3.951 -5.342	1.00	58.18
	1435	03	NAG A	221	48.035	17.468	-3.342 -4.966	1.00 1.00	64.80 76.76
	1436	C4	NAG A	221	49.919	15.918	-4.908	1.00	84.55
	1437	04	NAG A	221	50.874	16.976	-5.150	1.00	121.48
45	1438 1439	C5	NAG A	221	50.354	14.610	-5.540	1.00	75.06
73	1440	O5 C6	NAG A	221 221	49.589 51.837	13.531 14.319	-4.944 5.314	1.00	65.34
	1441	06	NAG A	221	52.240	13.109	-5.314 -5.940	1.00 1.00	72.88 79.15
	1442	C1	NAG A	222	50.797	17.958	-6.068	1.00	145.53
50	1443	C2	NAG A	222	50.822	19.497	-5.910	1.00	155.10
50	1444	N2	NAG A	222	49.525	20.056	-6.240	1.00	159.26
	1445 1446	C7 O7	NAG A NAG A	222 222	48.710	20.465	-5.270	1.00	165.01
	1447	C8	NAG A	222	48.999 47.367	20.393 21.040	-4.072 -5.688	1.00	169.69
	1448	C3	NAG A	222	51.905	20.174	-6.746	1.00	162.00 158.11
55	1449	О3	NAG A	222	51.976	21.552	-6.412	1.00	158.38
	1450	C4	NAG A	222	53.236	19.510	-6.450	1.00	161.49
	1451 1452	O4 C5	NAG A	∠22	54.266	20.119	-7.216	1.00	161.28
	1453	O5	NAG A NAG A	222 222	53.108 52.123	18.028 17.403	-6.799 -5.946	1.00	162.76
60	1454	C6	NAG A	222	54.409	17.273	-6.600	1.00 1.00	157.35 163.69
	1455	O6	NAG A	222	54.197	15.869	-6.619	1.00	157.92
	1456	C1	NAG A	242	43.365	-3. 26 2	-14.810	1.00	13.23
	1457 1458	C2	NAG A	242	43.041	-2.260	-15.917	1.00	5.53
65	1458	N2 C7	NAG A NAG A	242 242	44.141	-1.343 -1.740	-16.143	1.00	9.70
	1460	07 07	NAG A	242 242	45.252 45.439	-1.749 -2.917	-16.754 -17.133	1.00 1.00	29.25
	1461	C8	NAG A	242	46.337	-0.695	-16.957	1.00	32.16 12.96
	1462	C3	NAG A	242	41.793	-1.489	-15.507	1.00	4.59
70	1463	O3	NAG A	242	41.435	-0.559	-16.510	1.00	15.24
70	1464	C4	NAG A	242	40.615	-2.416	-15.249	1.00	11.27

	1465 1466 1467	O4 C5 O5	NAG A NAG A NAG A	242 242 242	39.565 41.027 42.281	-1.641 -3.581 -4.195	-14.619 -14.306	1.00	13.74 16.30
5	1468 1469	C6 -	NAG A NAG A	242 242	40.007 39.736	-4.698 -5.116	-14.704 -14.278 -12.948	1.00 1.00 1.00	7.58 28.55 38.66
	1470	C1	NAG A	243	38.610	-1.048	-15.431	1.00	38.51
	1471	C2	NAG A	243	37.449	-0.610	-14.570	1.00	39.03
	1472	N2	NAG A	243	36.919	-1.742	-13.845	1.00	47.25
10	1473	C7	NAG A	243	36.991	-1.735	-12.517	1.00	62.38
	1474	O7	NAG A	243	37.502	-0.806	-11.885	1.00	63.20
	1475	C8	NAG A	243	36.416	-2.926	-11.769	1.00	77.74
15	1476	C3	NAG A	243	36.389	0.062	-15.450	1.00	52.71
	1477	O3	NAG A	243	35.272	0.474	-14.669	1.00	54.98
	1478	C4	NAG A	243	37.029	1.275	-16.133	1.00	40.14
13	1479	O4	NAG A	243	36.079	1.889	-17.033	1.00	74.71
	1480	C5	NAG A	243	38.284	0.828	-16.909	1.00	29.29
	1481	O5	NAG A	243	39.196	0.104	-16.046	1.00	36.06
20	1482	C6	NAG A	243	39.063	2.012	-17.448	1.00	35.70
	1483	O6	NAG A	243	40.407	1.653	-17.751	1.00	34.26
	1484	C1	MAN A	244	35.717	3.208	-16.771	1.00	75.57
	1485	C2	MAN A	244	35.709	4.009	-18.090	1.00	81.10
	1486	O2	MAN A	244	34.884	3.345	-19.043	1.00	66.91
	1487	C3	MAN A	244	35.181	5.431	-17.820	1.00	79.87
25	1488	03	MAN A	244	35.162	6.216	-19.009	1.00	58.10
	1489	C4	MAN A	244	33.782	5.322	-17.211	1.00	73.02
	1490	04	MAN A	244	33.238	6.611	-16.994	1.00	79.27
20	1491	C5	MAN A	244	33.918	4.560	-15.890	1.00	70.92
	1492	O5	MAN A	244	34.401	3.215	-16.159	1.00	80.43
	1493	C6	MAN A	244	32.626	4.463	-15.080	1.00	62.83
30	1494	O6	MAN A	244	31.720	3.523	-15.638	1.00	93.61
	1495	C1	NAG A	274	56.076	-21.009	-1.119	1.00	118.55
	1496	C2	NAG A	274	57.346	-21.243	-0.277	1.00	122.52
35	1497	N2	NAG A	274	58.518	-20.916	-1.059	1.00	104.98
	1498	C7	NAG A	274	59.434	-20.096	-0.559	1.00	87.55
	1499	O7	NAG A	274	59.341	-19.596	0.555	1.00	87.40
	1500	C8	NAG A	274	60.642	-19.783	-1.417	1.00	88.80
	1501	C3	NAG A	274	57.521	-22.673	0.320	1.00	134.44
	1502	O3	NAG A	274	58.252	-22.494	1.568	1.00	158.45
40	1503	C4	NAG A	274	56.155	-23.387	0.619	1.00	135.00
	1504	O4	NAG A	274	56.251	-24.825	0.491	1.00	133.45
	1505	C5	NAG A	274	55.035	-22.969	-0.345	1.00	136.04
45	1506	O5	NAG A	274	54.951	-21.543	-0.442	1.00	130.02
	1507	C8	NAG A	274	53.668	-23.483	0.076	1.00	139.67
	1508	O6	NAG A	274	52.628	-22.635	-0.387	1.00	144,24
45	1509	C1	FCA A	275	59.339	-23.324	1.916	1.00	166.18
	1510	C2	FCA A	275	59.905	-22.923	3.289	1.00	176.23
	1511	C3	FCA A	275	60.762	-21.695	3.251	1.00	178.46
50	1512	C4	FCA A	275	61.991	-21.833	2.283	1.00	172.76
	1513	C5	FCA A	275	61.389	-22.191	0.896	1.00	176.96
	1514	C6	FCA A	275	62.389	-22.620	-0.196	1.00	180.24
	1515	O2	FCA A	275	58.772	-22.721	4.211	1.00	187.28
	1516	O3	FCA A	275	61.269	-21.376	4.553	1.00	178.44
	1517	O4	FCA A	275	62.910	-22.849	2.754	1.00	169.66
55	1518	O5	FCA A	275	60.459	-23.282	0.968	1.00	169.81
	1519	C1	NAG A	276	57.235	-25.594	1.103	1.00	98.00
	1520	C2	NAG A	276	56.691	-27.020	1.226	1.00	98.05
	1521 1522 1523	N2 C7 O7	NAC A NAG A NAG A	276 276 276	55.572 54.356 54.123	27.068 -27.358 -27.596	2.154 1.694 0.498	1.00 1.00 1.00	97.91 98.05
60	1524	C8	NAG A	276	53.223	-27.391	2.716	1.00	98.12
	1525	C3	NAG A	276	57.782	-28.020	1.658	1.00	97.73
	1526	O3	NAG A	276	57.292	-29.346	1.498	1.00	98.00
65	1527 1528 1529	C4 O4 C5	NAG A NAG A NAG A	276 276 276	59.057 60.118 59.467	-27.855 -28.595 -26.388	0.815 1.409	1.00 1.00	98.03 97.83 98.08
	1530	O5	NAG A	276	58.367	-25.586	0.717	1.00	97.92
	1531	C6	NAG A	276	60.628	-26.186	0.218	1.00	98.07
	1532	O6	NAG A	276	60.565	-24.929	-0.248	1.00	97.94
70	1533 1534	C1 C2	NAG A	340 340	39.040 39.952	-24.929 -8.595 -9.673	-0.904 19.969 19.363	1.00 1.00 1.00	97.99 100.93 110.08

	1535 1536	N2 C7	NAG A NAG A	34 0 340	39.319 39.582	-10.976 -11.912	19.455 18.542	1.00	124.78 135.15
	1537 1538	07 ·	NAG A	340	40.340	-11.731	17.581	1.00	143.28
5	1539	C8 C3	NAG A NAG A	340	38.887	-13.255	18.716	1.00	133.94
	1540	<u> </u>	NAG A	340 340	41.289 42.244	-9.672	20.154	1.00	111.41
	1541	č4	NAG A	340	41.892	-10.545 -8.253	19.553	1.00	102.38
	1542	04	NAG A	340	42.980	-8.268	20.277 21.194	1.00	118.52
	1543	C5	NAG A	340	40.818	-7.251	20.750	1.00 1.00	138.80
10	1544	O5	NAG A	340	39.674	-7.325	19.890	1.00	112.80 95.92
	1545	Ç6	NAG A	340	41.276	-5.810	20.749	1.00	115.39
	1546	06	NAG A	340	40.167	-4.937	20.919	1.00	113.34
	1547 1548	C1	NAG A	366	26.559	-8.481	-3.518	1.00	137.03
15	1549	C2 N2	NAG A NAG A	366	25.744	-9.771	-3.450	1.00	148.09
10	1550	C7	NAG A	366 366	26.028 25.085	-10.464	-2.209	1.00	155.02
	1551	07	NAG A	366	23.951	-10.564 -10.097	-1.276 -1.415	1.00	162.56
	1552	C8	NAG A	366	25.455	-11.299	0.005	1.00 1.00	164.09
00	1553	СЗ	NAG A	366	26.084	-10.660	-4.651	1.00	163.28 155.95
20	1554	03	NAG A	366	25.247	-11.807	-4.658	1.00	159.81
	1555	C4	NAG A	366	25.893	-9.878	-5.955	1.00	160.49
	1556 1557	O4 C5	NAG A	366	26.355	-10.659	-7.048	1.00	169.57
	1558	O5	NAG A NAG A	366	26.666	-8.550	-5.904	1.00	155.12
25	1559	C6	NAG A	366 366	26.272 26.413	-7.789 -7.679	-4.739 7.400	1.00	140.93
	1560	O6	NAG A	366	26.023	-7.679 -6.364	-7.123	1.00	152.76
	1561	CB	VAL B	1	4.75≥	40.855	-6.753 51.137	1.00 1.00	149.51
	1562	CG1	VAL B	1	5.003	40.880	49.633	1.00	126.57 131.97
20	1563	CG2	VAL B	1	3.866	42.021	51.535	1.00	130.09
30	1564	C	VAL B	1	5.086	38.381	51.284	1.00	100.44
	1565 1566	0	VAL B	1	6.179	38.608	50.764	1.00	97.65
	1567	N CA	VAL B VAL B	1	3.657	39.534	52.971	1.00	122.36
	1568	N N	PRO B	1 2	4.091 4.743	39.511 37.150	51.550	1.00	110.89
35	1569	CD	PRO B	2	3.715	36.682	51.681 52.617	1.00 1.00	91.57
	1570	CA	PRO B	2	5.701	36.083	51.401	1.00	86.81 92.03
	1571	CB	PRO B	2	5.219	34.937	52.280	1.00	92.13
	1572	ÇG	PRO B	2	4.469	35.618	53.356	1.00	98.41
40	1573	C	PRO B	2	5.482	35.783	49.928	1.00	104.42
40	1574 1575	0 N	PRO B GLN B	2	4.381	35.956	49.405	1.00	108.80
	1576	CA	GLN B	3 3	6.522	35.337	49.251	1.00	115.31
	1577	CB	GLN B	3	6.395 7.319	35.044 35.945	47.839 47.050	1.00	118.75
	1578	CG	GLN B	3	6.978	37.381	47.261	1.00 1.00	132.23 134.41
45	1579	CD	GLN B	3	5.850	37.837	46.374	1.00	126.94
	1580	OE1	GLN B	3	4.815	37.173	46.271	1.00	124.90
	1581	NE2	GLN B	3	6.038	38.982	45.724	1.00	122.46
	1582 1583	C	GLN B	3	6.793	33.624	47.639	1.00	113.83
50	1584	0 N	GLN B Lys b	3	7.983	33.320	47.488	1.00	116.50
-	1585	ČA	LYS B	4 4	5.812 6.188	32.736 31.357	47.641	1.00	104.77
	1586	CB	LYS B	4	4.972	30.448	47.465 47.319	1.00 1.00	92,78
	1587	CG	LYS B	4	3.816	31.031	46.558	1.00	100.70 119.63
	1588	CD	LYS B	4	2.912	29.900	46.094	1.00	129.60
55	1589	CE	LYS B	4	1.591	30.427	45.556	1.00	131.81
	1590	NZ	LYS B	4	0.528	29.403	45.762	1.00	129.85
	1591 1592	C	LYS B	4	7.093	31.230	46.253	1.00	81.27
	1593	N	LYS B PRO B	4 5	6.904	31.908	45.239	1.00	74.91
60	1594	CD	PRO B	5	8.133 8.529	30.392 29.619	46.370	1.00	75.63
	1595	CA	PRO B	5	9.074	30.177	47.557 45.271	1.00	71.19
	1596	CB	PRO B	5	10.020	29.110	45.820	1.00 1.00	65.65 54.74
	1597	CG	PRO B	5	9.982	29.343	47.268	1.00	65.46
65	1598	C	PRO B	5	8.255	29.650	44.097	1.00	64.33
65	1599	0	PRO B	5	7.090	29.277	44.255	1.00	65.82
	1600 1601	N	LYS B	6	8.858	29.608	42.923	1.00	65.65
	1602	CA CB	LYS B Lys b	6	8.152	29.109	41.762	1.00	62.04
	1603	CG	LYS B	6 6	7.636 6.697	30.279	40.927	1.00	55.18
70	1604	CD	LYS B	6	5.394	29.866 30.661	39.817 39.855	1.00	89.38
				-	U.UUT		U8.033	1.00	97.54

	1605	CE	LYS B	6 -	4.431	30.196	38.756	1.00	92.63
	1606	ŃZ	LYS B	6	3.107	30.872	38.837	1.00	79.21
	1607	C	LYS B	6	9.121	28.262	40.961	1.00	65.56
5	1608 1609	O N	LYS B VAL B	6	10.042	28.789	40.325	1.00	67.90
,	1610	CA	VAL B	7 7	8.931	26.946	41.015	1.00	70.60
	1611	CB	VAL B	7	9.803 9.507	26.041 24.560	40.280	1.00	65.28
	1612	CG1	VAL B	7	10.356	23.663	40.595 39.694	1.00 1.00	57.35
	1613	CG2	VAL B	7	9.806	24.266	42.064	1.00	39.82
10	1614	C	VAL B	7	9.621	26.268	38.785	1.00	63.76 60.19
	1615	0	VAL B	7	8.498	26.325	38.280	1.00	56.68
	1616 1617	N	SER B	8	10.736	26.423	38.087	1.00	44.71
	1618	CA CB	SER B SER B	8 8	10.719	26.639	36.656	1.00	31.26
15	1619	OG OG	SER B	8	11.396 12.802	27.952 27.750	36.318	1.00	41.26
	1620	Č	SER B	8	11.540	27.750 25.504	36.214 36.055	1.00 1.00	36.80
	1621	0	SER B	8	12.480	25.002	36.675	1.00	48.76 52.73
	1622	N	LEU B	9	11.202	25.094	34.844	1.00	48.97
20	1623	CA	LEU B	9	11.947	24.009	34.225	1.00	39.06
20	1624 1625	CB CG	LEU B	9	11.000	22.902	33.735	1.00	33 73
	1626	CD1	LEU B LEU B	9 9	9.752	22.521	34.533	1.00	40.03
	1627	CD2	LEU B	9	9.198 10.071	21.252 22.302	33.933	1.00	39.96
	1628	c c	LEU B	9	12.764	24.50 2	35.993 33.041	1.00 1.00	58.00
25	1629	0	LEU B	9	12.353	25.413	32.317	1.00	33.09 31.06
	1630	N.	ASN B	10	13.930	23.908	32.848	1.00	19.95
	1631	CA	ASN B	10	14.768	24.262	31.721	1.00	20.51
	1632 1633	CB CG	ASN B ASN B	10	15.833	25.276	32.096	1.00	41.33
30	1634	OD1	ASN B	10 10	16.763	25.559 26.031	30.942	1.00	52.07
	1635	ND2	ASN B	10	16.325 18.048	25.031 25.263	29.890	1.00	83.63
	1636	C	ASN B	10	15.446	23.008	31.119 31.211	1.00 1.00	49.68
	1637	0	ASN B	10	16.375	22.497	31.843	1.00	34.87 40.39
35	1638	N	PRO B	11	15.025	22.518	30.034	1.00	43.40
33	1639 1640	CD	PRO B	11	15.817	21.532	29.277	1.00	30.44
	1641	CA CB	PRO B PRO B	11	13.956	23.087	29.197	1.00	20.84
	1642	CG	PRO B	11 11	14.085 15.604	22.307 21.988	27.918	1.00	36.80
	1643	Č	PRO B	11	12.572	22.964	27.879 29.819	1.00 1.00	28.71
40	1644	0	PRO B	11	12.312	22.023	30.566	1.00	34.02 49.37
	1645	N	PRO B	12	11.663	23.896	29.482	1.00	30.69
	1646	CD	PRO B	12	11.938	24.837	28.384	1.00	30.68
	1647 1648	CA CB	PRO B PRO B	12	10.268	24.026	29.945	1.00	24.81
45	1649	CG	PRO B	12 12	9.668 10.861	25.062	28.995	1.00	34.63
	1650	Č	PRO B	12	9.452	25.893 22.761	28.607	1.00	49.64
	1651	Ō	PRO B	12	8.4 6 5	22.654	29.981 30.716	1.00 1.00	29.55 28.29
	1652	N	TRP B	13	9.873	21.802	29.176	1.00	38.99
50	1653	CA	TRP B	13	9.188	20.527	29.057	1.00	44.73
<i>3</i> 0	1654 1655	CB	TRP B	13	9.904	19.706	27.996	1.00	44.13
	1656	CG CD2	TRP B	13 13	10.282	20.578	26.874	1.00	32.01
	1657	CE2	TRP B	13	9.428 10.213	21.507 22.177	26.210	1.00	33.06
	1658	CE3	TRP B	13	8.069	21.841	25.247 26.335	1.00	37.35
55	1659	CD1	TRP B	13	11.520	20.712	26.306	1.00 1.00	32.11 30.68
	1660	NE1	TRP B	13	11.487	21.675	25.330	1.00	32.77
	1661	CZ2	TRP 8	13	9.686	23.160	24.411	1.00	42.92
	1662 1663	CZ3 CH2	TRP B TRP B	13	7.545	22.816	25.507	1.00	36.94
60	1664	C	TRP B	13 13	8.354 9.079	23.466	24.553	1.00	51.15
- •	1665	ŏ	TRP B	13	10.070	19.747 19.236	30.356 30.866	1.00	42.74
	1666	N	ASN B	14	7.862	19.660	30.879	1.00 1.00	27.87
	1667	CA	ASN B	14	7.609	18.933	32.107	1.00	39.20 42.44
65	1668	CB	ASN B	14	6.354	19.469	32.774	1.00	50.46
U)	1669	CG	ASN B	14	5.119	19.130	32.010	1.00	49.15
	1670 1671	OD1 ND2	ASN B	14	4.967	19.509	30.852	1.00	79.01
	1672	C ND2	ASN B ASN B	14 14	4.221	18.402	32.649	1.00	57.09
	1673	ŏ	ASN B	14	7.427 7.263	17.455 16.635	31.790	1.00	43.98
70	1674	N	ARG B	15	7.443	17.126	32.683 30.507	1.00 1.00	61.67
								1.00	44.77

	1675 1676	CA CB	ARG B	15 15	7.293	15.749	30.065	1.00	37.62
	1677	CG	ARG B	15	6.053 4.972	15.588	29.197	1.00	37.39
	1678	CD	ARG B	15	3.826	16.603 16.330	29.455	1.00	44.80
5	1679	NE	ARG B	15	3.226	15.032	28.510 28.791	1.00	56.59
	1680	CZ	ARG B	15	2.570	14.311	27.883	1.00 1.00	41.31
	1681	NH1	ARG B	15	2.435	14.759	26.639	1.00	40.12
	1682	NH2	ARG B	15	2.033	ເວ. ເວ5	28.246	1.00	57.43
10	1683	С	ARG B	15	8.522	15.500	29.221	1.00	28.82 31.33
10	1684	0	ARG B	15	8.737	16.159	28.202	1.00	34.58
	1685	N	ILE B	16	9.328	14.535	29.621	1.00	29.80
	1686	CA	ILE B	16	10.540	14.286	28.872	1.00	46.54
	1687 1688	CB	ILE B	16	11.728	14.912	29.604	1.00	56.61
15	1689	CG2 CG1	ILE B	16	11.405	16.370	29.923	1.00	58.31
10	1690	CD1	ILE B	16	11.988	14.150	30.9-2	1.00	61.86
	1691	Č,	ILE B	16 16	13.106 10.813	14.716	31.753	1.00	58.95
	1692	ŏ	ILE B	16	10.303	12.811 11.952	28.652	1.00	43.09
	1693	N	PHE B	17	11.619	12.532	29.383 27.634	1.00	46.04
20	1694	CA	PHE B	17	12.001	1:67	27.303	1.00	34.79
	1695	СВ	PHE B	17	12.605	11.118	25.894	1.00 1.00	46.60
	1696	CG	PHE B	17	11.585	11.032	24.793	1.00	38.91
	1697	CD1	PHE B	17	11.845	11.607	23.549	1.00	49.23 47.72
25	1698	CD2	PHE B	17	10.387	10.354	24.982	1.00	39.73
25	1699	CE1	PHE B	17	10.931	11.520	22.512	1.00	39.05
	1700	CE2	PHE B	17	9.465	10.258	23.957	1.00	33.44
	1701	cz	PHE B	17	9.736	10.840	22.713	1.00	50.08
	1702 1703	C	PHE B	17	13.028	10.639	28.305	1.00	53.02
30	1703	Ň	PHE B LYS B	17	13.828	11.405	28.859	1.00	46.68
20	1705	CA	LYS B	18 18	12.996	9.330	28.536	1.00	49.36
	1706	CB	LYS B	18	13.942 13.694	8.691 7.183	29.439	1.00	46.09
	1707	ČĞ	LYS B	18	14.791	6.380	29.470 30.134	1.00	30.09
	1708	CD	LYS B	18	14,541	4.890	29.967	1.00 1.00	62.01
35	1709	CE	LYS B	18	15.591	4.051	30.696	1.00	69.67 79.54
	1710	NZ	LYS B	18	16.966	4.233	30.147	1.00	7 8.34 74.39
	1711	С	LYS B	18	15.363	8.964	28.946	1.00	45.81
	1712	0	LYS B	18	15.641	8.877	27.761	1.00	48.24
40	1713	N	GLY B	19	16.261	9.305	29.860	1.00	54.24
40	1714 1715	CA	GLY B	19	17.634	9.564	29.470	1.00	48.03
	1716	C	GLY B	19	17.942	11.011	29.142	1.00	57.65
	1717	Ň	GLY B GLU B	19 20	19.110	11.364	28.964	1.00	57.96
	1718	CA	GLU B	20	16.916 17.142	11.855	29.050	1.00	59.66
45	1719	CB	GLU B	20	15.900	13.269 13.889	28.754	1.00	58.50
	1720	CG	GLU B	20	15.444	13.180	28.106 26.834	1.00	70.52
	1721	CD	GLU B	20	14.502	14.026	25.992	1.00 1.00	82.41 79.78
	1722	OE1	GLU B	20	13.490	14.527	26.550	1.00	67.98
50	1723	OE2	GLU B	20	14.786	14.176	24.776	1.00	80.75
50	1724	C	GLU B	20	17.474	14.021	30.046	1.00	52.56
	1725	0	GLU B	20	17.266	13.492	31.143	1.00	35.18
	1726 1727	N	ASN B	21	17.999	15.244	29.920	1.00	59.52
	1727	CA	ASN B	21	18.344	16.072	31.085	1.00	47.35
55	1729	CB CG	ASN B ASN B	21	19.753	16.640	30.956	1.00	30.47
55	1730	OD1	ASN B	21	20.784	15.572	30.658	1.00	55.82
	1731	ND2	ASN B	21 21	20.688 21.772	14.447	31.168	1.00	46.16
	1732	C	ASN B	21	17.383	15.924 17.239	29.835	1.00	67.36
	1733	Ō	ASN B	21	16.866	17.784	31.261 30.292	1.00 1.00	40.95
60	1734	N	VAL B	22	17.152	17.619	32.507	1.00	70.03 25.27
	1735	CA	VAL B	22	16.276	18.735	32.829	1.00	32.44
	1736	CB	VAL B	22	14.824	18.247	33.003	1.00	20.08
	1737	CG1	VAL B	22	14.692	17.429	34.270	1.00	24.18
65	1738	CG2	VAL B	22	13.882	19.426	33.061	1.00	36.02
UJ	1739	C	VAL B	22	16.775	19.385	34.139	1.00	43.21
	1740 1741	0	VAL B	22	17.327	18.710	35.003	1.00	49.24
	1741	N CA	THR B THR B	23	16.583	20.689	34.289	1.00	39.88
	1742	CB	THR B	23	17.030	21.383	35.489	1.00	33.49
70	1744	OG1	THR B	23 23	18.165	22.352	35.174	1.00	34.45
				٠.	19.216	21.655	34.493	1.00	42.02

	1745	CG2	THR B	23	18.693	22.967	36.456	1.00	50.00
	1746	Ç	THR B	23	15.931	22.190	36.167	1.00	52.09 43.19
	1747	<u>o</u> .	THR B	23	15.405	23.157	35.608	1.00	46.71
5	1748 1749	N CA	LEU B LEU B	24	15.591	21.797	37.383	1.00	44.29
,	1750	CB	LEU B LEU B	24 24	14.581 13.911	22.521	38.131	1.00	54.45
	1751	ČĠ	LEU B	24	13.237	21.596 20.376	39.141 38.519	1.00	48.21
	1752	CD1	LEU B	24	12.426	19.622	39.562	1.00 1.00	51.83 56.70
10	1753	CD2	LEU B	24	12.329	20.835	37.415	1.00	69.70
10	1754	C	LEU B	24	15.255	23.676	38.858	1.00	60.50
	1755 1756	0 N	LEU B THR B	24	16.299	23.494	39.482	1.00	84.20
	1757	CA	THR B	25 25	14.669 15.238	24.865 26.025	38.771 39.439	1.00	56.15
	1758	CB	THR B	25	15.715	27.055	38.435	1.00 1.00	48.18 36.73
15	1759	OG1	THR B	25	16.498	26.395	37.429	1.00	43.20
	1760	CG2	THR B	25	16.584	28.095	39.134	1.00	58.01
	1761 1762	C O	THR B	25	14.228	26.659	40.374	1.00	55.18
	1763	N	THR B CYS B	25 26	13.051 14.700	26.810	40.019	1.00	39.05
20	1764	ċ.	CYS B	26	13.866	27.010 27.603	41.571 42.608	1.00 1. 0 0	69.20
	1765	С	CYS B	26	14.115	29.091	42.752	1.00	77.69 84.84
	1766	0	CYS B	26	15.186	29.501	43.193	1.00	95.13
	1767	CB	CYS B	26	14.146	26.925	43.947	1.00	70.99
25	1768 1769	SG N	CYS B	26	12.878	27.161	45.240	1.00	87.46
23	1770	CA	ASN B ASN B	27 27	13.127	29.898	42.378	1.00	94.31
	1771	CB	ASN B	27	13.234 14.182	31.349 31.917	42.491	1.00	97.02
	1772	CG	ASN B	27	13.616	31.796	41.409 39.988	1.00 1.00	104.76
••	1773	OD1	ASN B	27	12.599	31.141	39.748	1.00	106.25 109.42
30	1774	ND2	ASN B	27	14.293	32.434	39.035	1.00	104.71
	1775	C	ASN B	27	11.848	31.975	42.388	1.00	95.21
	1776 1777	0 N	ASN B GLY B	27	10.979	31.462	41.684	1.00	83.43
	1778	ČA	GLY B	28 28	11.639 10.354	33.069 33.753	43.112	1.00	106.07
35	1779	Č.	GLY B	28	10.354	34.992	43.101 43.966	1.00 1.00	127.70 138.06
	1780	0	GLY B	28	10.631	34.879	45.182	1.00	143.08
	1781	N	ASN B	29	10.341	36.173	43.362	1.00	142.87
	1782 1783	CA	ASN B	29	10.498	37.424	44.099	1.00	153.48
40	1784	CB CG	ASN B ASN B	29	9.350	37.669	45.082	1.00	152.59
	1785	OD1	ASN B	29 29	9.535 10.508	38.959 39.679	45.876	1.00	158.12
	1786	ND2	ASN B	29	8.607	39.253	45.675 46.772	1.00 1.00	156.21 158.95
	1787	С	ASN B	29	11.787	37.198	44.865	1.00	161.65
AE	1788	0	ASN B	29	11.820	37.250	46.094	1.00	164.05
45	1789 1790	N CA	ASN B	30	12.842	36.920	44.109	1.00	173.43
	1790	CB	ASN B ASN B	30	14.136	36.629	44.690	1.00	183.92
	1792	CG	ASN B	30 30	15.174 16.451	36.378 35.752	43.593	1.00	190.23
	1793	OD1	ASN B	30	16.552	35.752 35.442	44.136 45.325	1.00 1.00	197.43 203.09
50	1794	ND2	ASN B	30	17.431	35.555	43.262	1.00	200.85
	1795	Ç	ASN B	30	14.653	37.685	45.639	1.00	186.26
	1796	0	ASN B	30	14.262	38.855	45.593	1.00	185.38
	1797 1798	N GA	PHE B	31	15.547	37.235	46.501	1.00	188.59
55	1799	CB	PHE B PHE B	31 31	16.173 15.485	38.036	47.500	1.00	194.52
	1800	ča	PHE B	31	15.971	37.780 38.766	48.8-\1 49.886	1.00	203.03
	1801	CD1	PHE B	31	15.408	40.027	49.940	1.00 1.00	210.47 216.06
	1802	CD2	PHE B	31	16.993	38.456	50.730	1.00	211.10
60	1803	CE1	PHE B	31	15.861	40.961	50.804	1.00	222.00
00	1804 1805	CE2 CZ	PHE B	31	17.485	39.387	51.600	1.00	215.51
	1806	C C	PHE B PHE B	31 31	16.924 17.640	40.643	51.640	1.00	219.04
	1807	ŏ	PHE B	31	17.649 18.344	37.672 37.980	47.559 48.535	1.00	191.71
	1808	Ň	PHE B	32	18.115	36.994	46.535 46.528	1.00 1.00	197.27 183.37
65	1809	CA	PHE B	32	19.516	36.543	46.471	1.00	176.18
	1810	CB	PHE B	32	20.457	37.696	46.108	1.00	171.85
	1811	CG CD1	PHE B	32	20.693	38.668	47.204	1.00	170.32
	1812 1813	CD1 CD2	PHE B PHE B	32	21.637	38.396	48.187	1.00	169.89
70	1814	CE1	PHE B	32 32	19.977 21.868	39.859 39.200	47.276	1.00	168.03
		- •		٠.	£1.000	39.298	49.221	1.00	164.25

	1815	CE2	PHE B	32-	20.201	40.765	48.308	1.00	160.78
	1816 1817	CZ C	PHE B PHE B	32	21.145	40.483	49.282	1.00	159.57
	1818	ŏ	PHE B	32 32	19.870	35.945	47.824	1.00	175.68
5	1819	Ň	GLU B	33	21.029 18.872	35.946 35.409	48.235	1.00	173.43
_	1820	CA	GLU B	33	19.012	34.712	48.474 49.721	1.00	177.15
	1821	СВ	GLU B	33	17.859	35.035	50.674	1.00 1.00	177.13
	1822	CG	GLU B	33	18.021	34.459	52.073	1.00	179.86
10	1823	CD	GLU B	33	19.050	35.206	52.898	1.00	176.70 173.43
10	1824	OE1	GLU B	33	19.758	36.067	52.334	1.00	173.17
	1825 1826	OE2	GLU B	33	19.151	34.929	54.111	1.00	172.06
	1827	C	GLU B	33	18.966	33.237	49.329	1.00	175.21
	1828	Ň	VAL B	33 34	18.622 19.311	32.361	50.122	1.00	174.80
15	1829	CA	VAL B	34	19.336	32.998 31.679	48.071	1.00	172.32
	1830	CB	VAL B	34	20.040	31.769	47.454 46.083	1.00	166.26
	1831	CG1	VAL B	34	20.242	30.393	45.487	1.00 1.00	167.66 171.78
	1832	CG2	VAL B	34	19.234	32.658	45.147	1.00	171.78
20	1833	Ç	VAL B	34	19.997	30.573	48.274	1.00	160.12
20	1834	0	VAL B	34	19.643	29.405	48,137	1.00	161.37
	1835 1836	N OA	SER B	35	20.953	30.940	49.117	1.00	154.76
	1837	CA CB	SER B SER B	35	21.668	29.962	49.933	1.00	144.31
	1838	OG OG	SER B	35 35	22.442	30.673	51.049	1.00	145.69
25	1839	č	SER B	35	21.565 20.772	31.183 28.897	52.038 50.555	1.00	143.47
	1840	ŏ	SER B	35	21.184	27.749	50.555 50.708	1.00	136.95
	1841	N	SER B	36	19.547	29.269	50.912	1.00 1.00	135.37 130.67
	1842	CA	SER B	36	18.623	28.328	51.542	1.00	127.00
20	1843	CB	SER B	36	17.944	28.990	52.748	1.00	133.26
30	1844	og	SER B	36	17.047	30.017	52.345	1.00	123.80
	1845 1846	C	SER B	36	17.545	27.766	50.615	1.00	123.00
	1847	0 N	SER B THR B	36	16.620	28.481	50.222	1.00	128.61
	1848	ČA	THR B	37 37	17.657 16. 67 5	26.480	50.282	1.00	107.86
35	1849	CB	THR B	37	17.089	25.821 25.793	49.426 47.928	1.00	88.91
	1850	OG1	THA B	37	17.358	27.116	47.445	1.00 1.00	87.15 64.20
	1851	CG2	THR B	37	15.955	25.213	47.103	1.00	90.90
	1852	C	THR B	37	16.469	24.376	49.854	1.00	86.86
40	1853	0	THR B	37	17.427	23.669	50.168	1.00	83.90
40	1854 1855	N	LYS B	38	15.212	23.948	49.845	1.00	82.11
	1856	CA CB	LYS B LYS B	38	14.835	22.596	50.224	1.00	83.86
	1857	CG	LYS B	38 38	13.885 14.442	22.630 22.010	51.427	1.00	86.79
	1858	CD	LYS B	38	15.694	22.734	52.699 53.185	1.00	100.07
45	1859	CE	LYS B	38	16.039	22.305	54.602	1.00 1.00	104.27 97.90
	1860	NZ	LYS B	38	14.882	22.578	55.510	1.00	91.89
	1861	Č	LYS B	38	14.115	21.953	49.051	1.00	82.06
	1862	0	LYS B	38	13.147	22.520	48.545	1.00	72.96
50	1863 1864	N CA	TRP B	39	14.579	20.784	48.613	1.00	82.25
50	1865	CA CB	TRP B TRP B	39	13.915	20.097	47.508	1.00	66.31
	1866	CG	TRP B	39 39	14.922 15.429	19.675	46.449	1.00	58.26
	1867	CD2	TRP B	39	14.789	20.832	45.665	1.00	63.66
	1868	· CE2	TRP B	39	15.607	21.453 22.534	44.542 44.139	1.00	65.27
55	1869	CE3	TRP B	39	13.605	21,201	43.841	1.00 1.00	67.87 51.05
	1870	CD1	TRP B	39	16.574	21.541	45.891	1.00	62.46
	1871	NE1	TRP B	39	16.690	22.565	44.977	1.00	57.52
	1872	CZ2	TRP B	39	15.277	23.364	43.061	1.00	59.34
60	1873 1874	CZ3 CH2	TRP B	39	13.280	22.023	42.775	1.00	59.55
00	1875	C	TRP B	39 39	14.114	23.093	42.395	1.00	51.52
	1876	ŏ	TRP B	39	13.113 13.484	18.888 18.191	47.971	1.00	57.60
	1877	Ň	PHE B	40	11.993	18.652	48.920 47.304	1.00	57.66 54.40
	1878	CA	PHE B	40	11.149	17.534	47.671	1.00 1.00	54.42 62.10
65	1879	CB	PHE B	40	9.926	18.018	48.449	1.00	62.19 54.85
	1880	CG	PHE B	40	10.262	18.678	49.745	1.00	59.54
	1881	CD1	PHE B	40	10.602	20.025	49.783	1.00	63.79
	1882 1883	CD2	PHE B	40	10.310	17.934	50.920	1.00	65.98
70	1884	CE1 CE2	PHE B	40 40	10.988	20.623	50.981	1.00	81.46
, ,	1007	CEZ	PHE B	40	10.696	18.518	52.122	1.00	72.69
				,					

	1885 1886	cz c	PHE B	40°	11.039	19.863	52.154	1.00	78.47
	1887	ŏ:	PHE B PHE B	40 40	10.688	16.728	46.476	1.00	68.64
	1888	Ň	HIS B	40 41	9.920 11.157	17.217	45.650	1.00	78.19
5	1889	CA	HIS B	41	10.778	15.487 14.593	46.396 45.314	1.00	72.46
	1890	СВ	HIS B	41	11.988	13.804	45.314 44.833	1.00	69.06
	1891	CG	HIS B	41	11.706	12.972	43.630	1.00 1.00	61.71
	1892	CD2	HIS B	41	12.491	12.132	42,921	1.00	66.30
10	1893	ND1	HIS B	41	10.476	12.970	43.011	1.00	62.70 68.58
10	1894	CE1	HIS B	41	10.517	12.161	41.967	1.00	82.82
	1895	NE2	HIS B	41	11.728	11.640	41.890	1.00	79.59
	1896 1897	C	HIS B	41	9.713	13.641	45.839	1.00	66.17
	1898	O N	HIS B ASN B	41	9.971	12.842	46.727	1.00	64.30
15	1899	CA	ASN B	42 42	8.511 7.423	13.726	45.288	1.00	75.54
	1900	CB	ASN B	42	7.739	12.877 11.397	45.751	1.00	79.71
	1901	CG	ASN B	42	7.203	10.871	45.530 44.210	1.00 1.00	78.21
	1902	OD1	ASN B	42	6.080	11.203	43.803	1.00	78.51 76.64
20	1903	ND2	ASN B	42	8.001	10.027	43.560	1.00	77.12
20	1904	C	ASN B	42	7.183	13.113	47.236	1.00	79.13
	1905	0	ASN B	42	6.754	12.203	47.958	1.00	64.42
	1906 1907	N CA	GLY B	43	7.478	14.330	47.692	1.00	81.21
	1908	C	GLY B	43	7.276	14.662	49.091	1.00	80.48
25	1909	ŏ	GLY B	43 43	8.459 8.452	14.460	50.020	1.00	64.04
	1910	Ň	SER B	44	5.45Z 5.472	14.985 13.719	51.123	1.00	63.95
	1911	CA	SER B	44	10.655	13.449	49.573 50.387	1.00 1.00	59.76
	1912	CB	SER B	44	11.191	12.034	50.114	1.00	64.76 70.69
20	1913	OG	SER B	44	10.248	11.045	50.502	1.00	89.71
30	1914	C	SER B	44	11.758	14.454	50.134	1.00	65.31
	1915 1916	0	SER B	44	12.038	14.802	48.993	1.00	76.25
	1917	N CA	LEU B LEU B	45 45	12.386	14.914	51.209	1.00	65.35
	1918	CB	LEU B	45 45	13.471 13.917	15.877 16.337	51.100	1.00	61.98
35	1919	ČĠ	LEV B	45	15.182	17.202	52.496 52.529	1.00	65.46
	1920	CD1	LEU B	45	14.971	18.471	51.691	1.00 1.00	79.05 77.35
	1921	CD2	LEU B	45	15.526	17.548	53.971	1.00	72.35
	1922	C	LEU B	45	14.663	15.278	50.351	1.00	60.60
40	1923 1924	O N	LEU B	45	15.109	14.168	50.638	1.00	63.58
40	1925	CA	SER B SER B	46 46	15.167	16.015	49.374	1.00	61.57
	1926	CB	SER B	46	16.315 16.247	15.564	48.608	1.00	73.03
	1927	ŌĞ	SER B	46	17.386	16.120 15. 7 37	47.186 46.432	1.00 1.00	77.22
	1928	С	SER B	46	17.569	16.083	49.302	1.00	90.60 80.37
45	1929	0	SER B	46	17.499	16.999	50.129	1.00	76.01
	1930	N	GLJ B	47	18.710	15.493	48.969	1.00	84.85
	1931 1932	CA	GLU B	47	19.974	15.930	49.548	1.00	84.12
	1933	CB CG	GLU B GLU B	47	21.027	14.827	49.429	1.00	87.82
50	1934	CD	GLU B	47 47	20.659 20.468	13.538	50.145	1.00	101.06
	1935	OE1	GLU B	47	20.638	13.733 14.876	51. 637 52.113	1.00 1.00	111.75
	1936	OE2	GLU B	47	20.148	12.744	52.329	1.00	115.76
	1937	С	GLU B	47	20.468	17.212	48.886	1.00	12.59 82.42
55	1938	0	GLU B	47	21.259	17.951	49.455	1.00	91.17
33	1939	N	GLU B	48	19.971	17.458	47.675	1.00	78.36
	1940 1941	CA CB	GLJ B	48	20.339	18.649	46.918	1.00	77.76
	1942	CG	GLU B	48	19.624	18.652	45.569	1.00	83.13
	1943	CD	GLU B	48 48	19.932 21.376	19.876	44.726	1.00	92.74
60	1944	OE1	GLU B	48	21.677	19.914 19.317	44.265 43.203	1.00	101.93
	1945	OE2	GLU B	48	22.204	20.531	44.975	1.00 1.00	102.91
	1946	C	GLU B	48	19.970	19.916	47.686	1.00	108.55 77.31
	1947	0	GLU B	48	18.853	20.040	48.204	1.00	74.82
65	1948	N	THR B	49	20.900	20.864	47.749	1.00	78.12
UJ.	1949 1950	CA CB	THR B	49	20.659	22,107	48.475	1.00	81.85
	1951	CB OG1	THR B THR B	49 40	21.526	22.184	49.748	1.00	83.91
	1952	CG2	THR B	49 49	22.684 20.726	21.353	49.593	1.00	88.24
	1953	c	THR B	49	20.726	21.743 23.390	50.961 47.680	1.00	75.28
70	1954	0	THR B	49	20.664	24.481	48.208	1.00 1.00	82.91 84.53
									J-1.33

	1955 1956 1957	N CA CB	ASN B ASN B ASN B	50 ⁻ 50 50	21.296 21.491 22.483	23.273 24.455	46.425 45.592	1.00 1.00	89.01 90.45
5	1958 1959	CG OD1	ASN B ASN B	50 50	22.910 22.449	24.139 25.375 26.482	44.463 43.697 43.971	1.00 1.00 1.00	96.17 111.81 112.79
	1960 1961 1962	ND2 C O	ASN B ASN B ASN B	50 50 50	23.798 20.123 19.208	25.190 24.856 24.033	42.727 45.013 44.942	1.00 1.00 1.00	110.81 89.21 94.63
10	1963 1964 1965	N CA CB	SER B SER B SER B	51 51 51	19.976 18.724 18.820	26.118 26.613 28.123	44.625 44.045	1.00 1.00	84.28 84.66
	1966 1967 1968	OG C	SER B SER B	51 51	20.000 18.387	28.461 25.940	43.846 43.134 42.699	1.00 1.00 1.00	90.77 104.30 77.58
15	1969 1970	O N CA	SER B SER B SER B	51 52 52	17.312 19.313 19.108	26.150 25.133 24.441	42.126 42.195 40.934	1.00 1.00 1.00	52.63 74.45 62.55
	1971 1972 1973	CB OG C	SER B SER B SER B	52 52 52	20.120 20.003 19.243	24.930 26.329 22.934	39.907 39.742 41.098	1.00 1.00 1.00	56.77 76.18
20	1974 1975 1976	O N CA	SER B LEU B LEU B	52 53 53	20.327 18.133	22.425 22.229	41.391 40.915	1.00 1.00	61.53 66.28 56.00
25	1977 1978 1979	CB CG CD1	LEU B LEU B	53 53	18.102 16.789 16.530	20.778 20.323 18.816	41.014 41.642 41.653	1.00 1.00 1.00	42.82 35.21 46.47
25	1980 1981	CD2 C	LEU B LEU B	53 53 53	17.775 15.337 18.236	18.057 18.539 20.189	42.111 42.565 39.627	1.00 1.00 1.00	51.40 29.95 40.92
30	1982 1983 1984	O N CA	LEU B ASN B ASN B	53 54 54	17.347 19.353 19.593	20.336 19.524 18.921	38.801 39.372 38.068	1.00 1.00 1.00	59.69 53.72 63.37
	1985 1986 1987	CB CG OD1	ASN B ASN B ASN B	54 54 54	21.064 21.475 20.985	19.074 20.516 21.239	37.686 37.562 36.691	1.00 1.00 1.00	66.79 81.16
35	1988 1989 1990	ND2 C O	ASN B ASN B ASN B	54 54 54	22.372 19.205	20.952 17.444	38.439 37.989	1.00 1.00	89.84 99.57 68.27
	1991 1992	N CA	ILE B	55 55	19.398 18.643 18.242	16.681 17.061 15.689	38.935 36.849 36.596	1.00 1.00 1.00	72.52 66.50 55.12
40	1993 1994 1995	CB CG2 CG1	ILE B ILE B ILE B	55 55 55	16.744 16.431 15.952	15.574 14.175 15.909	36.310 35.822 37.577	1.00 1.00 1.00	34.50 22.09 32.78
	1996 1997 1998	CD1 C O	ILE B ILE B ILE B	55 55 55	14.466 19.012 18.806	15.688 15.235 15.751	37.459 35.371 34.276	1.00 1.00 1.00	38.73 57.07 69.88
45	1999 2000 2001	N CA CB	VAL B VAL B VAL B	56 56 56	19.910 20.719 22.202	14.277 13.795 13.797	35.560 34.450	1.00 1.00	58.62 65.98
50	2002 2003 2004	CG1 CG2 C	VAL B VAL B	56 56	23.047 22.573	13.490 15.146	34.826 33.609 35.401	1.00 1.00 1.00	58.88 54.44 58.22
50	2005 2006	0 N	VAL B VAL B ASN B	56 56 57	∠0.326 20.232 20.103	12.401 11.468 12.272	33.984 34.782 32.678	1.00 1.00 1.00	71.96 82.07 70.61
55	2007 2008 2009	CA CB CG	ASN B ASN B ASN B	57 57 57	19.704 20.879 22.082	11.006 10.028 10.573	32.081 32.084 31.331	1.00 1.00 1.00	79.87 88.09 104.06
	2010 2011 2012	OD1 ND2 C	ASN B ASN B ASN B	57 57 57	21.990 23.220 18.532	10.934 10.640 10.441	30.151 32.013 32.865	1.00 1.00 1.00	109.39 110.76 77.25
60	2013 2014 2015	O N CA	ASN B ALA B ALA B	57 58 58	18.597 17.463 16.246	9.335 11.229 10.872	33.403 32.916 33.629	1.00 1.00	83.22 69.58
	2016 2017 2018	CB C O	ALA B ALA B ALA B	58 58	15.101 15.854	11.748 9.399	33.155 33.519	1.00 1.00 1.00	67.83 70.80 68.71
65	2019 2020	N CA	LYS B LYS B	58 59 59	15.912 15.472 15.035	8.790 8.837 7.452	32.455 34.655 34.742	1.00 1.00 1.00	63.76 62.18 62.15
7 0	2021 2022 2023	CB CD	LYS B LYS B LYS B	59 59 59	15.688 17.214 17.816	6.774 6.849 6.471	35.943 35.933 37.277	1.00 1.00 1.00	77.31 89.39 86.69
70	2024	CE	LYS B	59	19.320	6.717	37.280	1.00	83.05

2027 O LYS B 59 13.062 8.707 35.128 1.00 2028 N PHE B 60 12.813 6.486 35.016 1.00 2030 CB PHE B 60 11.380 6.608 35.014 1.00 2031 CG PHE B 60 10.857 5.310 34.915 1.00 2032 CD1 PHE B 60 10.808 4.884 33.480 1.00 2033 CD2 PHE B 60 19.917 4.149 33.072 1.00 2034 CE1 PHE B 60 9.837 5.216 32.533 1.00 2035 CE2 PHE B 60 9.977 4.826 31.96 1.00 2036 CZ PHE B 60 11.092 4.089 30.801 1.00 2037 C PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 10.203 7.639 7.7058 1.00 2039 N GLU B 61 12.097 6.503 7.7517 1.00 2040 CA GLU B 61 12.097 6.503 39.751 1.00 2041 CB GLU B 61 13.190 6.038 39.668 1.00 5.00 2043 CD GLU B 61 13.190 6.038 39.668 1.00 5.00 2044 OE1 GLU B 61 13.368 3.844 38.362 1.00 2045 CG GLU B 61 13.368 3.847 38.362 1.00 2046 C GLU B 61 12.459 3.888 37.861 1.00 10 2047 O GLU B 61 12.459 3.888 37.861 1.00 10 2048 N ASP B 62 12.459 3.888 37.861 1.00 10 2049 CA ASP B 62 12.579 9.007 38.174 1.00 7.7058 1.00 2051 CG ASP B 62 12.579 9.007 38.174 1.00 7.7058 1.00 2055 O ASP B 62 12.579 9.007 38.174 1.00 7.7058 1.00 10 2056 N SER B 63 9.076 11.029 37.311 1.00 7.7058 1.00 10 2057 CA SER B 63 10.391 10.440 37.533 1.00 6.00 30 2054 C ASP B 62 12.599 9.007 38.174 1.00 7.7058 1.00 10 2058 CB SER B 63 8.157 10.038 38.669 1.00 5.00 2059 OG SER B 63 8.157 10.038 38.669 1.00 5.00 2050 C SER B 63 8.571 11.353 38.669 1.00 5.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.669 1.00 6.00 2060 C SER B 63 8.571 11.353 38.777 1.00 650	
2027 O LYS B 59 13.062 8.707 35.128 1.00 2028 N PHE B 60 12.813 6.486 35.016 1.00 2030 CB PHE B 60 11.380 6.608 35.244 1.00 2031 CG PHE B 60 10.657 5.310 34.915 1.00 2031 CG PHE B 60 10.808 4.884 33.480 1.00 2032 CD1 PHE B 60 10.808 4.884 33.480 1.00 2033 CD2 PHE B 60 9.837 5.216 33.453 1.00 2033 CD2 PHE B 60 9.837 5.216 33.533 1.00 2035 CE2 PHE B 60 9.837 5.216 33.533 1.00 2036 CZ PHE B 60 11.092 4.089 30.801 1.00 2036 CZ PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.002 37.639 37.058 1.00 2036 CZ PHE B 60 11.002 37.639 37.058 1.00 2036 CZ PHE B 60 11.3097 6.503 37.517 1.00 2034 CD GLU B 61 12.044 6.763 38.944 1.00 E 2040 CA GLU B 61 12.044 6.763 38.944 1.00 E 2041 CB GLU B 61 13.190 6.038 39.668 1.00 2042 CG GLU B 61 13.190 6.038 39.668 1.00 2042 CG GLU B 61 13.396 3.847 38.362 1.00 10 2045 CD GLU B 61 13.368 3.847 38.362 1.00 10 2045 CD GLU B 61 13.368 3.847 38.362 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2046 C GLU B 61 12.459 3.188 37.861 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2046 C G GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045 CD GLU B 61 12.459 3.187 37.811 1.00 10 2045	80.45
5 2029 CA PHE B 60 11.380 6.608 35.016 1.00 2031 CG PHE B 60 10.657 5.310 34.915 1.00 2032 CD1 PHE B 60 10.808 4.884 33.480 1.00 2032 CD1 PHE B 60 10.808 4.884 33.480 1.00 2033 CD2 PHE B 60 11.919 4.1149 33.072 1.00 2033 CD2 PHE B 60 12.068 3.753 31.739 1.00 2035 CE2 PHE B 60 12.068 3.753 31.739 1.00 2035 CE2 PHE B 60 12.068 3.753 31.739 1.00 2036 CZ PHE B 60 9.977 4.826 31.196 1.00 2036 CZ PHE B 60 11.092 4.089 30.801 1.00 2037 C PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.166 6.982 6.6893 1.00 2039 N GLU B 61 12.097 6.503 37.517 1.00 2040 CA GLU B 61 12.097 6.503 37.517 1.00 2041 CB GLU B 61 13.190 6.038 39.668 1.00 2042 CG GLU B 61 13.190 6.038 39.668 1.00 2042 CG GLU B 61 13.368 3.847 38.362 1.00 11 2044 OE1 GLU B 61 13.368 3.847 38.362 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2048 N ASP B 62 12.579 9.007 38.174 1.00 6 6 2050 CB ASP B 62 15.963 10.452 38.299 1.00 5 5 2050 CB ASP B 62 15.963 10.257 36.923 1.00 7 7 2055 O DASP B 62 15.963 10.257 36.923 1.00 7 7 2055 O DASP B 62 15.963 10.257 36.923 1.00 7 7 2055 O DASP B 62 15.963 10.257 36.923 1.00 7 2055 O DASP B 62 15.963 10.391 10.440 37.533 1.00 5 2056 C ASP B 62 11.366 11.151 38.094 1.00 55 2056 C ASP B 62 11.366 11.359 38.462 1.00 55 2056 N SER B 63 9.076 11.029 37.311 1.00 55 2056 N SER B 63 9.076 11.029 37.311 1.00 55 2056 O C SER B 63 9.076 11.029 37.311 1.00 55 2056 O C SER B 63 9.076 11.029 37.311 1.00 55 2056 O C SER B 63 9.048 10.990 39.666 1.00 55 2050 C SER B 63	56.91
2030 CB PHE B 60 11.380 8.603 35.244 1.00 2031 CG PHE B 60 10.8657 5.310 34.915 1.00 2032 CD1 PHE B 60 10.808 4.884 33.480 1.00 1.00 2033 CD2 PHE B 60 19.837 5.216 32.533 1.00 2034 CE1 PHE B 60 12.068 3.753 31.739 1.00 2035 CE2 PHE B 60 9.837 5.216 32.533 1.00 2036 CZ PHE B 60 11.092 4.089 30.801 1.00 2037 C PHE B 60 11.092 4.089 30.801 1.00 2037 C PHE B 60 11.166 6.962 6.6693 1.00 2037 C PHE B 60 11.166 6.962 6.6693 1.00 6 2038 N GLU B 61 12.097 6.503 37.558 1.00 6 2040 CA GLU B 61 12.097 6.503 37.557 1.00 6 2041 CB GLU B 61 13.190 6.038 39.668 1.00 6 2042 CG GLU B 61 13.077 4.505 39.705 1.00 10 2043 CD GLU B 61 13.368 3.847 38.362 1.00 10 2043 CD GLU B 61 13.368 3.847 38.362 1.00 10 2044 OE1 GLU B 61 13.368 3.847 38.362 1.00 10 2045 OE2 GLU B 61 12.459 3.187 37.811 1.00 10 2046 C GLU B 61 12.459 3.187 37.811 1.00 10 2046 C GLU B 61 12.366 3.988 37.861 1.00 10 2047 O GLU B 61 12.366 3.988 37.861 1.00 10 2046 C GLU B 61 12.459 3.187 37.811 1.00 10 2046 C GLU B 61 12.459 3.187 37.811 1.00 10 2046 C GLU B 61 12.366 3.988 37.861 1.00 10 2046 C GLU B 61 12.459 3.187 37.811 1.00 10 2046 C GLU B 61 11.814 8.747 40.277 1.00 7 2048 N ASP B 62 12.579 9.007 38.174 1.00 7 2048 N ASP B 62 12.589 9.007 38.174 1.00 7 2048 N ASP B 62 12.589 10.452 38.299 1.00 55 2050 CB ASP B 62 13.720 11.010 37.306 1.00 55 2050 CB ASP B 62 13.780 37.744 1.00 7 2055 OC B ASP B 62 13.780 37.744 1.00 7 2055 OC B ASP B 62 13.780 37.744 1.00 7 2055 OC B ASP B 62 13.780 37.744 1.00 65 2055 OC A SER B 63 9.076 11.029 37.311 1.00 55 2055 OC A SER B 63 9.076 11.029 37.311 1.00 55 2050 CG SER B 63 8.557 10.038 36.669 1.00 55 2050 OG SER B 63 8.551 11.353 38.717 1.00 56 2062 N GLY B 64 7.439 12.135 38.717 1.00 56 2063 N GLY B 64 7.439 12.135 38.717 1.00 56 2063 N GLY B 64 7.439 12.135 38.717 1.00 56 2063 N GLY B 64 7.439 12.135 38.717 1.00 56 2063 N GLY B 64 7.439 12.135 38.717 1.00 56 2063 N GLY B 64 7.439 12.135 38.717 1.00 56 2063 N GLY B 64 7.439 12.135 38.717 1.00 56 2063 N GLY B 64 7.439 12.135 38.717 1.00 56 2063 N GLY B 64 7.439 12.135 38.717 1	72.49 42.51
2031 CG PHE B 60 10.808 4.884 33.480 1.00 2032 CD1 PHE B 60 11.919 4.149 33.072 1.00 10 2034 CE1 PHE B 60 9.837 5.216 32.533 1.00 2035 CE2 PHE B 60 9.877 4.826 31.196 1.00 2036 CZ PHE B 60 9.977 4.826 31.196 1.00 2037 C PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.66 6.962 6.693 1.00 6 2038 O PHE B 60 10.203 7.639 .7.058 1.00 6 2039 N GLU B 61 12.097 6.503 37.517 1.00 7 2040 CA GLU B 61 12.097 6.503 37.517 1.00 7 2041 CB GLU B 61 13.190 6.038 39.668 1.00 6 2042 CG GLU B 61 13.077 4.505 39.705 1.00 10 2043 CD GLU B 61 13.368 3.847 38.362 1.00 10 2044 OE1 GLU B 61 13.368 3.847 38.362 1.00 10 2045 CD GLU B 61 12.459 3.887 38.362 1.00 11 2046 C GLU B 61 12.459 3.887 37.811 1.00 11 2047 O GLU B 61 12.136 8.267 39.188 1.00 7 2048 N ASP B 62 12.579 9.007 38.174 1.00 7 2050 CB ASP B 62 13.720 11.010 37.306 1.00 5 2051 CG ASP B 62 15.963 10.277 36.923 1.00 5 2052 OD1 ASP B 62 15.963 10.277 36.923 1.00 5 2053 OD2 ASP B 62 11.366 11.356 38.941 1.00 5 2056 N SER B 63 9.076 11.038 36.669 1.00 5 2057 CA SER B 63 9.076 11.223 38.291 1.00 5 2058 CB SER B 63 9.076 11.038 36.669 1.00 5 2060 C SER B 63 8.676 9.678 35.341 1.00 75 2063 CA CLU B 64 7.439 12.135 38.717 1.00 55 2063 CA CLU B 64 7.439 12.135 38.717 1.00 55	48.10
2032 CD1 PHE B 60 11.919 4.149 33.072 1.00 2033 CD2 PHE B 60 9.837 5.216 32.533 1.00 2035 CE2 PHE B 60 12.068 3.753 31.739 1.00 2036 CZ PHE B 60 11.092 4.089 30.801 1.00 2037 C PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 11.092 4.089 30.801 1.00 2038 O PHE B 60 10.203 7.639 7.058 1.00 2039 N GLU B 61 12.097 6.503 77.557 1.00 2040 CA GLU B 61 12.097 6.503 77.557 1.00 2041 CB GLU B 61 13.077 4.505 39.765 1.00 2042 CG GLU B 61 13.077 4.505 39.765 1.00 2043 CD GLU B 61 13.368 3.847 38.362 1.00 2043 CD GLU B 61 13.368 3.847 38.362 1.00 2044 OE1 GLU B 61 14.506 3.988 37.861 1.00 2045 OE2 GLU B 61 12.459 3.187 37.811 1.00 2046 C GLU B 61 12.459 3.187 37.811 1.00 2047 O GLU B 61 12.136 8.267 39.188 1.00 2048 N ASP B 62 12.579 5.007 38.174 1.00 2050 CB ASP B 62 13.720 11.010 37.306 1.00 2051 CG ASP B 62 15.152 10.763 37.744 1.00 2052 OD1 ASP B 62 15.963 10.277 36.923 1.00 30 SER B 63 9.076 11.029 37.311 1.00 31 SER B 63 10.391 10.440 37.533 1.00 32 OOS CB SER B 63 8.157 10.038 38.669 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00 39.666 1.00	48.50
10 2033	64.06
2035 CE2 PHE B 60 9.977 4.826 31.196 1.00 1.2036 CZ PHE B 60 9.977 4.826 31.196 1.00 2.037 C PHE B 60 11.092 4.089 30.801 1.00 0.2037 C PHE B 60 11.166 6.962 6.693 1.00 0.2038 O PHE B 60 11.2097 6.503 7.5058 1.00 0.2040 CA GLU B 61 12.097 6.503 37.517 1.00 0.2041 CB GLU B 61 12.097 6.503 37.517 1.00 0.2041 CB GLU B 61 13.190 6.038 39.668 1.00 0.2042 CG GLU B 61 13.190 6.038 39.668 1.00 0.2043 CD GLU B 61 13.368 3.847 38.362 1.00 10.2043 CD GLU B 61 13.368 3.847 38.362 1.00 10.2045 OE2 GLU B 61 12.459 3.187 37.811 1.00 10.2045 OE2 GLU B 61 12.459 3.187 37.811 1.00 10.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.811 1.00 11.2047 O GLU B 61 12.459 3.187 37.311 1.00 11.2047 O GLU B 61 12.459 3.187 37.311 1.00 11.2047 O GLU B 61 12.459 3.187 37.344 1.00 6.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50.005 50	63.95 74.15
2036 CZ PHE B 60 11.092 4.089 30.801 1.00 62 2037 C PHE B 60 11.092 4.089 30.801 1.00 6 2038 C PHE B 60 11.166 6.962 .6.693 1.00 6 2038 C PHE B 60 10.203 7.639 .7.058 1.00 6 2040 CA GLU B 61 12.097 6.503 37.517 1.00 7 2041 CB GLU B 61 12.044 6.763 38.944 1.00 6 2042 CG GLU B 61 13.190 6.038 39.668 1.00 6 2042 CG GLU B 61 13.077 4.505 39.705 1.00 10 2043 CD GLU B 61 13.368 3.847 38.362 1.00 10 2044 OE1 GLU B 61 13.368 3.847 38.362 1.00 11 2045 OE2 GLU B 61 12.459 3.187 37.861 1.00 10 2046 C GLU B 61 12.459 3.187 37.861 1.00 10 2047 O GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.136 8.267 39.188 1.00 7 2048 N ASP B 62 12.579 9.007 38.174 1.00 7 2048 N ASP B 62 12.579 9.007 38.174 1.00 6 2050 CB ASP B 62 12.599 1.00 37.306 1.00 5 2051 CG ASP B 62 15.152 10.763 37.744 1.00 65 2051 CG ASP B 62 15.152 10.763 37.744 1.00 7 2055 OD1 ASP B 62 15.162 10.763 37.744 1.00 7 2055 OD1 ASP B 62 15.467 11.068 38.916 1.00 7 2055 OD ASP B 62 15.467 11.068 38.916 1.00 7 2055 O ASP B 62 15.467 11.068 38.916 1.00 55 2057 CA SER B 63 10.391 10.440 37.533 1.00 44 2057 CA SER B 63 10.391 10.440 37.533 1.00 44 2056 C SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.669 1.00 55 2059 OG SER B 63 8.157 10.038 36.6	62.10
2037 C PHE B 60 11.166 6.962 56.693 1.00 6 2 2 2 2 2 2 3 9 N GLU B 61 12.097 6.503 37.517 1.00 7 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	74.92
15 2038	69.78
2040 CA GLU B 61 12.097 6.503 37.517 1.00 7.2041 CB GLU B 61 13.190 6.038 38.944 1.00 8 2042 CG GLU B 61 13.190 6.038 39.668 1.00 9 2043 CD GLU B 61 13.368 3.847 38.362 1.00 10 2044 OE1 GLU B 61 13.368 3.847 38.362 1.00 10 2044 OE1 GLU B 61 14.506 3.988 37.861 1.00 10 2045 OE2 GLU B 61 12.459 3.187 37.861 1.00 10 2046 C GLU B 61 12.459 3.187 37.861 1.00 10 2047 O GLU B 61 12.136 8.267 39.188 1.00 7 2048 N ASP B 62 12.579 9.007 38.174 1.00 7 2048 N ASP B 62 12.579 9.007 38.174 1.00 6 2050 CB ASP B 62 13.720 11.010 37.306 1.00 5 2051 CG ASP B 62 13.720 11.010 37.306 1.00 5 2051 CG ASP B 62 15.152 10.763 37.744 1.00 7 2053 OD2 ASP B 62 15.963 10.277 36.923 1.00 7 2053 OD2 ASP B 62 11.366 11.151 38.094 1.00 50 2055 O ASP B 62 11.366 11.151 38.094 1.00 50 2055 O ASP B 62 11.366 11.151 38.094 1.00 50 2055 O ASP B 62 11.366 11.151 38.094 1.00 50 2056 N SER B 63 10.391 10.440 37.533 1.00 42 2057 CA SER B 63 9.076 11.029 37.311 1.00 55 2059 OG SER B 63 8.157 10.038 36.609 1.00 55 2059 OG SER B 63 8.511 11.353 38.669 1.00 44 2063 CA ASP B 64 7.439 12.135 38.717 1.00 56 2063 CA GLU B 64 7.439 12.135 38.717 1.00 56 2063 CA GLU B 64 7.439 12.135 38.717 1.00 56 2063 CA GLU B 64 7.439 12.135 38.717 1.00 56 2063	55.02
2041 CB GLU B 61 13.190 6.038 38.944 1.00 6.2042 CG GLU B 61 13.190 6.038 39.668 1.00 5.2043 CD GLU B 61 13.077 4.505 39.705 1.00 10.2044 OE1 GLU B 61 13.368 3.847 38.362 1.00 11.2045 OE2 GLU B 61 14.506 3.988 37.861 1.00 10.2046 C GLU B 61 12.459 3.187 37.811 1.00 10.2046 C GLU B 61 12.136 8.267 39.188 1.00 77.2048 N ASP B 62 12.579 9.007 38.174 1.00 77.2048 N ASP B 62 12.579 9.007 38.174 1.00 77.2048 N ASP B 62 12.579 9.007 38.174 1.00 77.2048 CA ASP B 62 12.599 1.00 55.2050 CB ASP B 62 13.720 11.010 37.306 1.00 55.2051 CG ASP B 62 15.152 10.763 37.744 1.00 77.2052 OD11 ASP B 62 15.467 11.068 38.916 1.00 57.2052 OD11 ASP B 62 15.467 11.068 38.916 1.00 88.2053 OD2 ASP B 62 15.963 10.277 36.923 1.00 77.2053 OD2 ASP B 62 11.366 11.151 38.094 1.00 77.2055 O ASP B 62 11.366 11.151 38.094 1.00 56.2056 N SER B 63 10.391 10.440 37.533 1.00 47.2057 CA SER B 63 9.076 11.029 37.311 1.00 56.2057 CA SER B 63 9.076 11.029 37.311 1.00 56.2057 CA SER B 63 9.076 11.029 37.311 1.00 56.2058 CB SER B 63 8.511 11.353 38.669 1.00 44.2062 N GLY B 64 7.439 12.135 38.717 1.00 56.2063 CA GLY B 64 7.439 12.135 38.717 1.00 56.2063 CA GLY B 64 7.439 12.135 38.717 1.00 56.2063 CA GLY B 64 7.439 12.135 38.717 1.00 56.2063	61.86 75.45
2042 CG GLU B 61 13.077 4.505 39.705 1.00 10 2043 CD GLU B 61 13.368 3.847 38.362 1.00 10 2044 OE1 GLU B 61 14.506 3.988 37.861 1.00 10 2045 OE2 GLU B 61 12.459 3.187 37.811 1.00 10 2046 C GLU B 61 12.136 8.267 39.188 1.00 7 2047 O GLU B 61 12.136 8.267 39.188 1.00 7 2048 N ASP B 62 12.579 5.007 38.174 1.00 7 2048 N ASP B 62 12.579 5.007 38.174 1.00 6 2050 CB ASP B 62 12.698 10.452 38.299 1.00 5 2051 CG ASP B 62 13.720 11.010 37.306 1.00 5 2052 OD1 ASP B 62 15.152 10.763 37.744 1.00 7 2053 OD2 ASP B 62 15.467 11.068 38.916 1.00 8 30 2054 C ASP B 62 15.467 11.068 38.916 1.00 8 30 2054 C ASP B 62 15.467 11.068 38.916 1.00 8 30 2055 O ASP B 62 11.366 11.151 38.094 1.00 5 2055 O ASP B 62 11.366 11.151 38.094 1.00 55 2056 N SER B 63 10.391 10.440 37.533 1.00 7 2057 CA SER B 63 10.391 10.440 37.533 1.00 44 2057 CA SER B 63 9.076 11.029 37.311 1.00 55 2058 CB SER B 63 9.076 11.029 37.311 1.00 55 2058 CB SER B 63 8.576 9.676 35.341 1.00 76 2060 C SER B 63 8.511 11.353 38.669 1.00 44 2062 N GLY B 64 7.439 12.135 38.717 1.00 55	83.97
2043 CD GLU B 61 13.368 3.847 38.362 1.00 10 2045 OE2 GLU B 61 14.506 3.988 37.861 1.00 10 2045 OE2 GLU B 61 12.459 3.187 37.811 1.00 10 2046 C GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.136 8.267 39.188 1.00 77 2048 N ASP B 62 12.579 5.007 38.174 1.00 77 2048 N ASP B 62 12.579 5.007 38.174 1.00 6 2050 CB ASP B 62 12.698 10.452 38.299 1.00 5 2051 CG ASP B 62 13.720 11.010 37.306 1.00 5 2052 OD1 ASP B 62 15.152 10.763 37.744 1.00 77 2053 OD2 ASP B 62 15.467 11.068 38.916 1.00 8 30 2054 C ASP B 62 15.467 11.068 38.916 1.00 8 30 2054 C ASP B 62 15.466 11.151 38.094 1.00 5 2055 O ASP B 62 15.466 11.151 38.094 1.00 5 2055 O ASP B 62 11.366 11.151 38.094 1.00 5 2055 O ASP B 62 11.366 11.151 38.094 1.00 5 2055 O ASP B 62 11.366 11.151 38.094 1.00 5 2056 N SER B 63 10.391 10.440 37.533 1.00 47 2057 CA SER B 63 9.076 11.029 37.311 1.00 55 2058 CB SER B 63 9.076 11.029 37.311 1.00 55 2058 CB SER B 63 8.576 9.676 35.341 1.00 77 2062 N GLY B 64 7.439 12.135 38.717 1.00 55 2063 CA GLY B 64 7.439 12.135 38.717 1.00 55 2063 CA GLY B 64 7.439 12.135 38.717 1.00 55 2063 CA GLY B 64 7.439 12.135 38.717 1.00 55 2063 CA GLY B 64 7.439 12.135 38.717 1.00 55 2063	96.33
2045 OE2 GLU B 61 14.506 3.988 37.861 1.00 10 2046 C GLU B 61 12.459 3.187 37.811 1.00 11 2047 O GLU B 61 12.136 8.267 39.188 1.00 7 2048 N ASP B 62 12.579 5.007 38.174 1.00 7 2050 CB ASP B 62 12.698 10.452 38.299 1.00 5 2051 CG ASP B 62 13.720 11.010 37.306 1.00 5 2052 OD1 ASP B 62 15.152 10.763 37.744 1.00 7 2053 OD2 ASP B 62 15.467 11.068 38.916 1.00 7 2053 OD2 ASP B 62 15.963 10.277 36.923 1.00 7 30 2054 C ASP B 62 15.963 10.277 36.923 1.00 7 2055 O ASP B 62 11.366 11.151 38.094 1.00 5 2056 N SER B 63 10.391 10.440 37.533 1.00 7 2057 CA SER B 63 10.391 10.440 37.533 1.00 41 2058 CB SER B 63 9.076 11.029 37.311 1.00 51 2058 CB SER B 63 8.157 10.038 36.609 1.00 51 2060 C SER B 63 8.517 10.038 36.609 1.00 51 2061 O SER B 63 9.048 10.900 39.666 1.00 52 2062 N GLY B 64 7.439 12.135 38.717 1.00 55	06.00
2046	10.30 09.44
2047 O GLU B 61 11.814 8.747 40.277 1.00 7 2048 N ASP B 62 12.579 9.007 38.174 1.00 7 25 2049 CA ASP B 62 12.698 10.452 38.299 1.00 5 2050 CB ASP B 62 13.720 11.010 37.306 1.00 5 2051 CG ASP B 62 15.152 10.763 37.744 1.00 7 2052 OD1 ASP B 62 15.152 10.763 37.744 1.00 7 2053 OD2 ASP B 62 15.963 10.277 36.923 1.00 7 2055 O ASP B 62 15.963 10.277 36.923 1.00 7 2055 O ASP B 62 11.366 11.151 38.094 1.00 5 2056 N SER B 63 10.391 10.440 37.533 1.00 4 2057 CA SER B 63 10.391 10.440 37.533 1.00 4 2058 CB SER B 63 9.076 11.029 37.311 1.00 5 2058 CB SER B 63 8.157 10.038 36.609 1.00 51 2060 C SER B 63 8.517 10.038 36.609 1.00 77 2061 O SER B 63 8.511 11.353 38.669 1.00 77 2062 N GLY B 64 7.439 12.135 38.717 1.00 55	11.21
25 2048 N ASP B 62 12.579 5.007 38.174 1.00 7 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	78.63
2050 CB ASP B 62 12.698 10.452 38.299 1.00 55 2051 CG ASP B 62 15.152 10.763 37.744 1.00 7 2052 OD1 ASP B 62 15.152 10.763 37.744 1.00 7 2053 OD2 ASP B 62 15.963 10.277 36.923 1.00 8 30 2054 C ASP B 62 15.963 10.277 36.923 1.00 7 2055 O ASP B 62 11.366 11.151 38.094 1.00 5 2056 N SER B 63 10.391 10.440 37.533 1.00 50 2057 CA SER B 63 9.076 11.029 37.311 1.00 50 2058 CB SER B 63 9.076 11.029 37.311 1.00 50 2059 OG SER B 63 8.157 10.038 36.609 1.00 50 2060 C SER B 63 8.517 10.038 36.609 1.00 50 2061 O SER B 63 8.511 11.353 38.669 1.00 40 2062 N GLY B 64 7.439 12.135 38.717 1.00 50	79.41
2051 CG ASP B 62 13.720 11.010 37.306 1.00 5 2052 OD1 ASP B 62 15.152 10.763 37.744 1.00 7 2053 OD2 ASP B 62 15.467 11.068 38.916 1.00 8 30 2054 C ASP B 62 15.963 10.277 36.923 1.00 7 2055 O ASP B 62 11.366 11.151 38.094 1.00 5 2056 N SER B 63 10.391 10.440 37.533 1.00 5 2057 CA SER B 63 9.076 11.029 37.311 1.00 5 2058 CB SER B 63 9.076 11.029 37.311 1.00 5 35 2059 OG SER B 63 8.157 10.038 36.609 1.00 51 2060 C SER B 63 8.517 10.038 36.609 1.00 51 2061 O SER B 63 8.511 11.353 38.669 1.00 44 2062 N GLY B 64 7.439 12.135 38.717 1.00 55	64.96 66.09
2052 OD1 ASP B 62 15.467 11.068 38.916 1.00 8 2053 OD2 ASP B 62 15.963 10.277 36.923 1.00 7 2053 OD2 ASP B 62 15.963 10.277 36.923 1.00 7 2055 O ASP B 62 11.366 11.151 38.094 1.00 52 2056 N SER B 63 10.391 10.440 37.533 1.00 42 2057 CA SER B 63 9.076 11.029 37.311 1.00 52 2058 CB SER B 63 8.157 10.038 36.609 1.00 52 2059 OG SER B 63 8.157 10.038 36.609 1.00 52 2060 C SER B 63 8.511 11.353 38.669 1.00 77 2061 O SER B 63 9.048 10.900 39.666 1.00 52 2062 N GLY B 64 7.439 12.135 38.717 1.00 55	8.67
2053 OD2 ASP B 62 15.963 10.277 36.923 1.00 7 2054 C ASP B 62 11.366 11.151 38.094 1.00 52 2055 O ASP B 62 11.227 12.325 38.442 1.00 52 2056 N SER B 63 10.391 10.440 37.533 1.00 42 2057 CA SER B 63 9.076 11.029 37.311 1.00 52 2058 CB SER B 63 8.157 10.038 36.609 1.00 52 2059 OG SER B 63 8.576 9.676 35.341 1.00 70 2060 C SER B 63 8.511 11.353 38.669 1.00 42 2061 O SER B 63 9.048 10.900 39.666 1.00 52 2062 N GLY B 64 7.439 12.135 38.717 1.00 55	2.63
30	5.98
2056 N SER B 63 10.391 10.440 37.533 1.00 40.2057 CA SER B 63 9.076 11.029 37.311 1.00 50.2058 CB SER B 63 8.157 10.038 36.609 1.00 50.2059 OG SER B 63 8.157 10.038 36.609 1.00 50.2050 C SER B 63 8.511 11.353 38.669 1.00 77.2061 O SER B 63 8.511 11.353 38.669 1.00 40.2060 C SER B 63 9.048 10.900 39.666 1.00 40.2062 N GLY B 64 7.439 12.135 38.717 1.00 50.2063	1.52
2057 CA SER B 63 9.076 11.029 37.331 1.00 43 2058 CB SER B 63 9.076 11.029 37.311 1.00 55 2059 OG SER B 63 8.157 10.038 36.609 1.00 55 2060 C SER B 63 8.676 9.676 35.341 1.00 77 2061 O SER B 63 8.511 11.353 38.669 1.00 44 2062 N GLY B 64 7.439 12.135 38.717 1.00 55	2.65 0.83
2058 CB SER B 63 8.157 10.038 36.609 1.00 55 2059 OG SER B 63 8.676 9.676 35.341 1.00 77 2061 O SER B 63 8.511 11.353 38.669 1.00 40 2062 N GLY B 64 7.439 12.135 38.717 1.00 55 2063 CA GLY B 64 7.439 12.135 38.717 1.00 55	7.35
2060 C SER B 63 8.676 9.676 35.341 1.00 56 2060 C SER B 63 8.511 11.353 38.669 1.00 46 2061 O SER B 63 9.048 10.900 39.666 1.00 56 2062 N GLY B 64 7.439 12.135 38.717 1.00 56	1.69
2060 C SER B 63 8.511 11.353 38.669 1.00 48 2061 O SER B 63 9.048 10.900 39.666 1.00 58 2062 N GLY B 64 7.439 12.135 38.717 1.00 56	9.14
2062 N GLY B 64 7.439 12.135 38.717 1.00 55	6.77 8.98
2063 CA GLV B 04 7.439 12.135 38.717 1.00 50	5.63
	0.75
40 2064 C GLY B 64 6.550 13.922 40.254 4.00	4.90
2005 O GLY B 64 6.405 14.721 39.327 1.00 56	7.89 5.67
2067 CA GLU B 65 6.456 14.260 41.536 1.00 63	3.70
2068 CB GH B 65 6.161 15.619 41.982 1.00 62	2.19
45 2069 CG GLU B 65 4715 16 899 43.009 1.00 58	3.85
2070 CD GLU B 65 3.957 16.719 44.960 1.00 74	1.39
2077 OE1 GLU B 65 4.578 16.285 45.968 1.00 90	5.38).14
2073 C GLU B 65 2.734 17.002 44.976 1.00 104	1.83
30 2074 O GLU B 65 8.084 15.718 42.598 1.00 58	3.45
2075 N TYR B 66 7.647 17.533 42.176 1.00 57	7.76
2076 CA TYR B 66 8.768 18.291 42.696 1.00 24).99 J.15
2078 CG TVB B 60 9.797 18.547 41.614 1.00 10).05
55 2079 CD1 TYR B 66 10.185 18.517 40.273 1.00 33	.40
2080 CE1 TYR B 66 10.957 15.427 20.776 1.00 44	.SI
2001 CD2 TYR B 66 11.794 17.042 41.841 1.00 54	.60 .50
2083 C7 TYR B 66 12.574 15.951 41.445 1.00 59	.78
60 2084 OH TYR B 66 12.154 15.150 40.405 1.00 62	.67
2085 C TVP R 66 12.075 40.013 1.00 60.	.36
2086 O TYR B 66 7.440 20.275 43.271 1.00 44	
2088 CA LYS B 67 8.888 20.006 44.380 1.00 55	.42 .20
65 2089 CB LYS B 67 7390 21.275 45.043 1.00 54.	
2090 CG LYS B 67 7.088 19.025 45.879 1.00 37.	.10
2091 CD LYS B 67 5,836 20.053 47,545 1.00 40.	
2092 CE LYS B 67 5.362 18.702 48.076 1.00 55.	
70 2094 C LYS B 67 4.355 18.855 49.172 1.00 79	
78. 79. 79. 79. 79. 79. 79. 79. 79. 79. 79	

	2095 2096	0	LYS B	67	10.222	20.891	46.730	1.00	
	2097	N CA	CYS B	68	10.161	22.924	45.761		80.11
	2098	Č.	CYS B CYS B	68	11.261	23.443	46.547		69.06
	5 2099	ŏ	CYS B	68	10.728	24.348	47.641		75.09 76.08
	2100	СВ	CYS B	68 68	9.543 12.231	24.682	47.671	1.00	78.03
	2101	SG	CYS B	68	11.523	24.217	45.665	1.00	71.35
	2102	N	GLN B	69	11.625	25.691 24.756	44.866	1.00	75.66
10	2103) 2104	CA	GLN B	69	11.233	25.600	48.527	1.00	80.08
1,	2104	CB CG	GLN B	69	10.612	24.728	49.635 50.712	1.00	74.62
	2106	CD	GLN B GLN B	69	10.067	25.488	51.859	1.00 1.00	70.96
	2107	OE1	GLN B	69	9.343	24.592	52.818	1.00	72.60 88.38
	2108	NE2	GLN B	69 69	9.406	23.363	52.720	1.00	85.19
15		С	GLN B	69	8.656 12.418	25.199	53.760	1.00	98.27
	2116	0	GLN B	69	13.519	26.356 25.819	50.212	1.00	78.27
	2111	N	HIS B	70	12.193	27.611	50.311	1.00	81.84
	2112 2113	CA	HIS B	70	13.252	28.398	50.577 51.183	1.00	82.10
20	2114	C3 C3	HIS B	70	13.822	29.437	50.192	1.00 1.00	85.15
	2115	CD2	HIS B HIS B	70	12.892	30.565	49.860	1.00	82.03
	2116	ND1	HIS B HIS B	70 70	12.763	31.800	50.398	1.00	93.26 95.48
	2117	CE1	HIS B	70 70	11.997 11.361	30.515	48.812	1.00	109.66
25	2118	NE2	HIS B	70	11.804	31.671	48.721	1.00	109.26
25		С	HIS B	70	12.735	32.468 29.044	49.672	1.00	109.02
	2120	0	HIS B	70	11.549	29.350	52.469	1.00	85.57
	2121 2122	N	GLN B	71	13.635	29.213	52.598 53.431	1.00	85.74
	2123	CA CB	GLN B	71	13.312	29.777	54.740	1.00 1.00	79.77
30	2124	CG	GLN B GLN B	71	14.619	30.126	55.465	1.00	80.82 89.59
	2125	CD	GLN B	71 71	14.460	30.447	56.945	1.00	103.30
	2126	OE1	GLN B	71	15.762 16.789	30.921	57.585	1.00	109.00
	2127	NE2	GLN B	71	15.726	30.220 32.120	57.542	1.00	100.56
35	2128 2129	C	GLN B	71	12.365	30.993	58.184	1.00	102.47
<i>J</i>	2130	0	GLN B	71	12.486	31.913	54.763 53.953	1.00	67.00
	2131	N GA	GLN B	72	11.432	30.978	55.715	1.00 1.00	42.78
	2132	CB	GLN B GLN B	72	10.460	32.063	55.922	1.00	69.70 70.51
40	2133	ČĞ	GLN B	72 72	11.188	33.388	56.149	1.00	78.43
40	2134	CD	GLN B	72	11.812 12.598	33.551	57.509	1.00	78.98
	2135	OE1	GLN B	72	13.532	34.838 35.065	57.593	1.00	95.13
	2136 2137	NE2	GLN B	72	12.223	35.700	56.807	1.00	97.37
	2137	C	GLN B	72	9.398	32.282	58.540 54.840	1.00	98.58
45	2139	0 N	GLN B	72	8.737	33.329	54.816	1.00 1.00	66.32
	2140	ÇA	VAL B VAL B	73	9.227	31.302	53.960	1.00	61.96 63.38
	2141	CB	VAL B	73 73	8.249	31.414	52.884	1.00	57.15
	2142	CG1	VAL B	73 73	8. 933 9.710	31.810	51.592	1.00	31.26
50	2143	CG2	VAL B	73	7.918	30.646 32.256	51.074	1.00	36.55
50	2144 2145	C	VAL B	73	7.552	30.075	50.585 52.663	1.00	50.56
	2146	O N	VAL B	73	8.148	29.022	52.896	1.00 1.00	59.51
	2147	ČA	ASN B	74	6.300	30.115	52.210	1.00	77.00
~-	2148	CB	asn b Asn b	74 74	5.534	28.892	51.965	1.00	61.46 68.17
5 5	2149	CG	ASN P	74	4.195 3.211	29.223	51.312	1.00	73.30
	2150	OD1	ASN B	74	2.787	29.829 29.182	52.267	1.00	72.42
	2151 2152	ND2	asn b	74	2.831	31.081	53.225	1.00	62.22
	2153	C	ASN B	74	6.251	27.885	52.014 51.066	1.00	85.31
60	2154	0 N	ASN B	74	7.342	28.142	50.543	1.00 1.00	73.92
	2155	ČA	GLU B GLU B	75	5.612	26.732	50.891	1.00	73.43 82.35
	2156	CB	GLU B	75 75	6.138	25.682	50.029	1.00	88.01
	2157	CG	GLU B	75 75	5.450 5.062	24.338	50.297	1.00	88.41
65	2158	CD	GLU B	75 75	5.962 5.673	23.548	51.490	1.00	102.21
UJ	2159	OE1	GLU B	75	4.497	22.053 21.692	51.358	1.00	103.43
	2160 2161	OE2	GLU B	75	6.622	21.242	51.118	1.00	95.26
	2162	C O	GLU B	75	5.844	26.073	51.493 48.592	1.00	104.69
	2163	N	GLU B SER B	75 70	4.760	26.580	48.287	1.00 1.00	85.00
70	2164	ČA	SER B	76 76	6.799	25.830	47.705	1.00	92.66 74.73
				76	6.597	26.136	46.299	1.00	74.73 64.93

	0405	~~	050.0						
	2165 2166	CB OG	SER B SER B	76- 76	7.811 7.884	25.716 24.300	45.474	1.00	65.57
	2167	č	SER B	76 76	7.86 4 5.392	25.350	45.366 45.802	1.00 1.00	53.84
_	2168	0	SER B	76	4.920	24,425	46.467	1.00	64.12 55.19
5	2169	N	GLU B	77	4.891	25.745	44.639	1.00	73.18
	2170	CA	GLU B	77	3.779	25.015	44.046	1.00	69.69
	2171 2172	CB CG	GLU B GLU B	77 77	3.077 2.498	25.874	42.993	1.00	59.63
	2173	CD	GLU B	77	1.820	27.169 28.000	43.535 42.462	1.00	89.51
10	2174	OE1	GLU B	77	1.798	27.557	41.295	1.00 1.00	107.00 103.77
	2175	OE2	GLU B	77	1.312	29.093	42.789	1.00	116.96
	2176	C	GLU B	77	4.246	23.698	43.437	1.00	63.68
	2177 2178	0 N	GLU B PRO B	77 78	5.367	23.648	42.922	1.00	69.58
15	2179	CD	PRO B	78	3.458 2.145	22.659 22.518	43.542 44.185	1.00 1.00	56.73
	2180	CA	PRO B	78	3.910	21.387	42.987	1.00	60.28 49.00
	2181	СВ	PRO B	78	2.760	20.438	43.304	1.00	42.75
	2182	ÇG	PRO B	78	2.141	21.046	44.534	1.00	68.49
20	2183 2184	C	PRO B PRO B	78 78	4.155 3.483	21.509 22.260	41.497	1.00	44.78
	2185	Ň	VAL B	79	5.137	20.766	40.795 41.024	1.00 1.00	52.51
	2186	CA	VAL B	79	5.486	20.745	39.616	1.00	34.40 23.08
	2187	CB	VAL B	79	6.779	21.527	39.364	1.00	17.91
25	2188 2189	CG1 CG2	VAL B	79	7.636	20.834	38.297	1.00	4.69
23	2190	C	VAL B VAL B	79 7 9	6.413 5.674	22.948 19.278	38.961	1.00	17.83
	2191	ŏ	VAL B	79	6.573	18.609	39.257 39.783	1.00 1.00	40.76
	2192	N	TYR B	80	4.831	18.773	38.362	1.00	37.75 43.38
30	2193	CA	TYR B	80	4.912	17.375	37.992	1.00	37.05
30	2194 2195	CB CG	TYR B TYR B	80	3.510	16.807	37.858	1.00	19.64
	2196	CD1	TYR B	80 80	2.736 1.881	16.988 18.084	39.122 39.293	1.00	52.81
	2197	CE1	TYR B	80	1.205	18.294	40.505	1.00 1.00	64.76 83.30
25	2198	CD2	TYR B	80	2.901	16.098	40.186	1.00	64.99
35	2199	CE2	TYR B	80	2.235	16.294	41.404	1.00	80.87
	2200 2201	CZ OH	TYR B TYR B	80 80	1.390 0.754	17.394	41.559	1.00	84.40
	2202	C,	TYR B	80	5.723	17.609 17.083	42.767 36.752	1.00 1.00	76.06
4.0	2203	Ö	TYR B	80	5.472	17.622	35.674	1.00	42.78 56.71
40	2204	N	LEU B	81	6.716	16.223	36.937	1.00	42.87
	2205 2206	CA CB	LEV B	81	7.615	15.798	35.878	1.00	47.81
	2207	CG	LEU B LEU B	81 81	9.049 10.151	15.953 15.383	36.360	1.00	39.60
	2208	CD1	LEU B	81	10.131	16.055	35.481 34.119	1.00 1.00	53.84 61.99
45	2209	CD2	LEU B	81	11.494	15.611	36.160	1.00	65.74
	2210	C	LEU B	81	7.312	14.328	35.562	1.00	60.00
	2211 2212	O N	LEU B	81	7.172	13.508	36.467	1.00	72.6 .
	2213	CA CA	GLU B	82 82	7.208 6.888	13.992 12.623	34.282 33.895	1.00 1.00	60.42
50	2214	СВ	GLU B	82	5.425	12.559	33.475	1.00	51.18 60.43
•	2215	CG	GLU B	82	4.967	11.207	32.988	1.00	75.17
	2216	CD	GLU B	82	3.453	11.151	32.824	1.00	92.83
	2217 2218	OE1 OE2	GLU B	82 82	2.880 2.839	12.091	32.219	1.00	98.53
55	2219	C	GLU B	82	7.778	10.166 12.089	33.301 32.780	1.00 1.00	97.49
	22 20	0	GLU B	82	7.734	12.564	31.645	1.00	49.31 54.46
	2221	N	VAL B	83	8.590	11.095	33.116	1.00	44.13
	2222 2223	CA CB	VAL B VAL B	83	9.512	10.492	32.158	1.00	51.30
60	2224	CG1	VAL B	83 83	10.656 11.654	9.749 9.218	32.862	1.00	44.14
	2225	CG2	VAL B	83	11.334	10.669	31.812 33.861	1.00 1.00	45.56 46.11
	2226	C	VAL B	83	8.820	9.488	31.246	1.00	55.74
	2227 2228	0	VAL B	83	8.110	8.609	31.713	1.00	73.69
65	2228	N CA	PHE B PHE B	84 84	9.051	9.608	29.945	1.00	53.23
	2230	ČB	PHE B	84	8.431 7.631	8.70 7 9.481	28.981 27.929	1.00 1.00	49.95
	2231	CG	PHE B	84	6.436	10.200	27.929 28.462	1.00	49.58 35.11
	2232	CD1	PHE B	84	6.570	11.175	29.423	1.00	52.71
70	2233 2234	CD2	PHE B	84	5.176	9.913	27.982	1.00	56.24
, 0	2234	CE1	PHE B	84	5.463	11.859	29.898	1.00	63.67

	2235 2236	CE2 CZ	PHE B PHE B	84 ⁻ 84	4.062 4.210	10.595 11.568	28.453 29.414	1.00	57.29
	2237	Č.	PHE B	84	9.495	7.935	28,238	1.00 1.00	52.51
_	2238	Ö	PHE B	84	10.696	8.144	28.444	1.00	56.77
5	2239	N	SER B	85	9.021	7.056	27.360	1.00	51.00 59.31
	2240	CA	SER B	85	9.856	6.236	26.496	1.00	53.43
	2241	CB	SER B	85	10.382	5.014	27.230	1.00	52.20
	2242	OG	SER B	85	11.313	4.342	26.403	1.00	68.06
10	2243 2244	C O	SER B	85	8.929	5.799	25.372	1.00	61.23
10	2244 2245	Ň	SER B ASP B	85 86	8.107	4.897	25.547	1.00	56.17
	2246	CA	ASP B	86 86	9.053 8.228	6.474 6.219	24.234	1.00	68.29
	2247	CB	ASP B	86	6.812	6.736	23.064 23.321	1.00 1.00	57.51
	2248	ČĞ	ASP B	86	5.802	6.181	22.336	1.00	51.72 90.19
15	2249	OD1	ASP B	86	6.002	6.371	21.113	1.00	100.01
	2250	OD2	ASP B	86	4.811	5.554	22.788	1.00	98.70
	2251	Ç	ASP B	86	8.868	6.974	21.897	1.00	57.18
	2252	0	ASP B	86	9.851	7.701	22.080	1.00	62.75
20	2253 2254	N	TRP B	87	8.330	6.799	20.699	1.00	51.37
20	2255	CA CB	TRP B	87 87	8.896	7.483	19.543	1.00	50.71
	2256	CG	TRP B	87 87	8.415 8.811	6.811	18.264	1.00	58.25
	2257	CD2	TRP B	87	10.032	5.379 4.880	18.134 17.562	1.00	53.11
	2258	CE2	TRP B	87	9.945	3.476	17.552	1.00 1.00	52.15
25	2259	CE3	TRP B	87	11.187	5.489	17.054	1.00	60.06 60.86
	2260	CD1	TRP B	87	8.060	4.285	18.452	1.00	44.63
	2261	NE1	TRP B	87	8.734	3.138	18.096	1.00	23.48
	2262	CZ2	TRP B	87	10.964	2.672	17.056	1.00	78.55
20	2263	CZ3	TRP B	87	12.197	4.691	16.561	1.00	84.54
30	2264	CH2	TRP B	87	12.077	3.294	16.565	1.00	87.37
	2265 2266	C	TRP B	87	8.545	8.982	19.495	1.00	42.37
	2267	0 N	TRP B	87	9.367	9.839	19.123	1.00	23.61
	2268	CA	LEU B	88 88	7.308 6.893	9.296 10.682	19.849	1.00	29.09
35	2269	CB	LEU B	88	5.817	10.844	19.837 18.777	1.00 1.00	31.21
	2270	CG	LEU B	88	6.167	10.869	17.290	1.00	33.13 18.54
	2271	CD1	LEU B	88	5.021	11.506	16.542	1.00	25.10
	2272	CD2	LEU B	88	7.449	11.594	16.959	1.00	4.59
40	2273	C	LEU B	88	6.348	11.083	21.182	1.00	40.21
40	2274	0	LEU B	88	5.517	10.381	21.783	1.00	42.92
	2275	N	LEU B	89	6.815	12.234	21.644	1.00	40.58
	2276 2277	CA CB	LEU B	89	6.369	12.780	22.912	1.00	31.34
	2278	CG	LEU B	89 89	7.514	12.805	23.921	1.00	33.17
45	2279	CD1	LEU B	89	7.202 5.821	13.378 12. 93 3	25.299	1.00	42.18
	2280	CD2	LEU B	89	8.282	12.923	25.763 26.264	1.00 1.00	52.47
	2281	C	LEU b	89	5.899	14.194	22.621	1.00	49.06 27.75
	2282	0	LEU B	89	6.617	14.973	21.947	1.00	5.35
50	2283	N	LEU B	90	4.703	14.517	23,109	1.00	4.73
50	2284	CA	LEU B	90	4.149	15.830	22.883	1.00	7.84
	2285	CB	LEU B	90	2.634	15.775	22.724	1.00	21.81
	2286	CG CD1	LEU B	90	2.032	17.148	22.410	1.00	21.45
	2287 2288		LEU B	90	2.511	17.587	21.026	1.00	29.29
55	2289	CD2 C	LEU B	90 90	0.521	17.103	22.464	1.00	15.21
	2290	Ö	LEU B	90	4.473 3.901	16.654 16.441	24.087	1.00	25.07
	2291	Ň	GLN E	91	5.382	.7.603	25.149 23.924	1.00 1.00	44.25
	2292	CA	GLN B	91	5.768	18.461	25.028	1.00	35.94 35.91
	2293	СВ	GLN B	91	7.273	18.707	24.955	1.00	17.00
60	2294	CG	GLN B	91	8.061	17.428	25.129	1.00	13.88
	2295	CD	GLN B	91	9.547	17.637	25.066	1.00	35.42
	2296	OE1	GLN B	91	10.092	18.074	24.040	1.00	18.59
	2297	NE2	GLN B	91	10.226	17.318	26.165	1.00	42.81
65	2298 2299	C	GLN B	91 01	4.995	19.781	25.025	1.00	36.56
55	2300	0 N	GLN B ALA B	91 92	4.606	20.285	23.966	1.00	49.74
	2301	ÇA	ALA B	92 92	4.761 4.054	20.335 21.607	26.212	1.00	35.59
	2302	CB	ALA B	92	2.628	21.607 21.377	26.313 26.734	1.00	43.59
	2303	Č	ALA B	92	4.719	22.580	26.734 27.283	1.00 1.00	28.50 53.87
70	2304	0	ALA B	92	5.250	22.184	28.318	1.00	53.87 69.37
				_				1.00	U8.3/

	2305 2306 2307	N CA CB	SER B SER B SER B	93 [.] 93 93	4.684 5.252	23.860 24.923	26. 932 27.761	1.00 1.00	68.52 64.18
	2308	OG	SER B	93	4.947 3.537	26.287 26.475	27.133	1.00	72.74
5	2309	Č.	SER B	93	4.593	24.849	26.986 29.128	1.00	77.53
	2310	Ö	SER B	93	5.200	25.163	30.143	1.00 1.00	56.86
	2311	N	ALA B	94	3.336	24.430	29.131	1.00	67.19 36.84
	2312	CA	ALA B	94	2.560	24.304	30.346	1.00	46.61
10	2313	СВ	ALA B	94	2.296	25.671	30.923	1.00	39.28
10	2314 2315	C	ALA B	94	1.248	23.611	29.999	1.00	57.58
	2316	Ň	ALA B GLU B	94 95	0.553	24.008	29.063	1.00	64.68
	2317	CA	GLU B	95	0.912 -0.311	22.571 21.824	30.754	1.00	65.01
	2318	CB	GLU B	95	-0.290	20.535	30.510 31.329	1.00 1.00	66.91
15	2319	CG	GLU B	95	0.872	19.619	30.950	1.00	69.50 64.00
	2320	CD	GLU B	95	0.886	18.326	31.738	1.00	82.38
	2321	OE1	GLU B	95	1.716	17.452	31.415	1.00	86.38
	2322	OE2	GLU B	95	0.075	18.181	32.678	1.00	93.94
20	2323 2324	CO	GLU B	95	-1.540	22.669	30. 83 1	1.00	68.95
20	2325	Ň	GLU B VAL B	95 96	-2.644	22.394	30.346	1.00	67.01
	2326	CA	VAL B	96	-1.345 -2.442	23.703 24.603	31.644	1.00	72.58
	2327	CB	VAL B	96	-3.012	24.282	.31.996 33.374	1.00	72.17
	2328	CG1	VAL B	96	-4.277	25.079	33.592	1.00 1.00	56.87
25	2329	CG2	VAL B	96	-3.280	22.788	33.489	1.00	54.83 38.14
	2330	Č	VAL B	96	-1.980	26.059	31.988	1.00	76.73
	2331	0	VAL B	96	-1.079	26.441	32.738	1.00	76.80
	2332 2333	N	VAL B	97	-2.611	26.867	31.141	1.00	80.52
30	2334	CA CB	VAL B VAL B	97	-2.258	28.271	30.996	1.00	82.56
50	2335	CG1	VAL B	97 97	-1.740 -1.543	28.546	29.562	1.00	85.79
	2336	CG2	VAL B	97	-0.429	30.029 27.803	29.341	1.00	102.89
	2337	C	VAL B	97	-3.420	29.216	29.334 31.283	1.00 1.00	95.31
~ ~	2338	0	VAL B	97	-4.591	28.885	31.041	1.00	82.63 75.81
35	2339	N	MET B	98	-3.073	30.394	31.807	1.00	84.13
	2340	CA	MET B	98	-4.050	31.442	32.112	1.00	91.67
	2341	CB	MET B	98	-3.430	32.509	33.020	1.00	102.42
	2342 2343	CG SD	MET B	98	-3.324	32.120	34.480	1.00	120.32
40	2344	CE	MET B MET B	98 98	-4.951 5.607	31.748	35.181	1.00	137.79
	2345	C	MET B	98	-5.607 -4.488	33.383 32.107	35.438	1.00	124.64
	2346	ŏ	MET B	98	-3.637	32.555	30.808 30.027	1.00 1.00	86.05
	2347	Ň	GLU B	99	-5.797	32.193	30.571	1.00	83.23 75.14
4.5	2348	CA	GLU B	99	-6.266	32.803	29.334	1.00	80.10
45	2349	СВ	GLU B	99	-7.745	33.156	29.408	1.00	83.15
	2350	CG	GLU B	99	-8.228	33.862	28.144	1.00	109.03
	2351 2352	CD OE1	GLU B	99	-9.693	34.250	28.204	1.00	121.43
	2353	OE2	GLU B	99	-10.084	34.917	29.189	1.00	131.12
50	2354	C	GLU B	99 99	-10.446 5.477	33.893	27.265	1.00	120.08
••	2355	ŏ	GLU B	95 95	-5.477 -5.371	34.059 34.955	29.019 29.846	1.00	76.85
	2356	Ň	GLY B	100	-4.915	34.113	27.818	1.00 1.00	76.94
	2357	CA	GLY B	100	-4.139	35.273	27.429	1.00	81.06 80.78
E E	2358	Ç	GLY B	100	-2.644	35.015	27.460	1.00	77.00
55	2359	0	GLY B	100	-1.877	35.674	26.752	1.00	79.67
	2360 2361	N CA	GLN B	101	-2.220	34.062	28.284	1.00	75.05
	2362	CA CB	GLN B GLN B	101	-0.798	33.729	28.370	1.00	78.99
	2363	CG	GLN B	101 101	-0.494 -0.561	32.996	29.682	1.00	84.76
60	2364	CD	GLN B	101	0.340	33.870 35.097	30.924	1.00	92.38
	2365	OE1	GLN B	101	-0.007	36.083	30.817 30.156	1.00 1.00	98.22 100.31
	2366	NE2	GLN B	101	1.509	35.036	31.456	1.00	92.08
	2367	С	GLN B	101	-0.351	32.876	27.178	1.00	65.25
65	2368	0	GLN B	101	-1.169	32.375	26.414	1.00	57.39
UJ	2369	N	PRO B	102	0.963	32.708	26.997	1.00	59.88
	2370 2371	CD	PRO B	102	2.093	33.382	27.653	1.00	62.83
	2372	CA CB	PRO B	102	1.422	31.901	25.868	1.00	59. 94
	2373	CG	PRO B PRO B	102 102	2.864	32.365	25.683	1.00	48.67
70	2374	č	PRO B	102	3.284 1.313	32.645 30.411	27.070	1.00	63.93
		_			1.010	30.411	26.120	1.00	60.51

	2375	0	PRO B	102	1.559	29.938	27.220	1.00	71.07
	2376	N	LEU B	103	0.926	29.686	25.081	1.00	66.31
	2377	CA	LEU B	103	0.780	28.238	25.119	1.00	56.78
5	2378 2379	CB	LEU B	103	-0.664	27.880	24.821	1.00	50.78
,	2380	CD1	LEU B	103 103	-0.974 -0.629	26.402 25.680	24.666	1.00	77.35
	2381	CD2	LEU B	103	-2.450	26.229	25.955 24.318	1.00	76.88
	2382	C	LEU B	103	1.703	27.688	24.030	1.00 1.00	77.48
	2383	0	LEU B	103	1.554	28.025	22.857	1.00	54.03 55.72
10	2384	N	PHE B	104	2.655	26.842	24.402	1.00	48.78
	2385	CA	PHE B	104	3.607	26.332	23.414	1.00	45.32
	2386	CB	PHE B	104	4.979	26.893	23.748	1.00	32.16
	2387 2388	CG CD1	PHE B	104	5.976	26.705	22.677	1.00	32.32
15	2389	CD2	PHE B	104 104	6.158	27.689 25.566	21.717	1.00	39.73
	2390	CE1	PHE B	104	6.770 7.123	27.544	22.641 20.708	1.00	39.96
	2391	CE2	PHE B	104	7.744	25.404	21.638	1.00 1.00	55.96 63.91
	2392	CZ	PHE B	104	7.923	26.404	20.673	1.00	61.86
20	2393	С	PHE B	104	3.700	24.805	23.299	1.00	42.46
20	2394	0	PHE B	104	4.206	24.140	24.199	1.00	46.85
	2395	N CA	LEU B	105	3.223	24.250	22.190	1.00	35.08
	2396 2397	CB	LEU B	105 105	3.277	22.811	22.006	1.00	22.82
	2398	CG	LEU B	105	1.999 0.804	22.311 22.355	21.356 22.298	1.00	37.29
25	2399	CD1	LEU B	105	-0.404	21.635	21.660	1.00 1.00	42.12 56.32
	2400	CD2	LEU B	105	1.196	21.673	23.579	1.00	54.72
	2401	С	LEU B	105	4.468	22.421	21.165	1.00	23.23
	2402	0	LEU B	105	5.055	23.250	20.476	1.00	30.46
30	2403	N	ARG B	106	4.833	21.149	21.226	1.00	15.51
30	2404 2405	CA CB	ARG B	106	5.990	20.674	20.475	1.00	30.48
	2406	CG	ARG B	106 106	7.249 8.540	21.056	. 21.243	1.00	25.17
	2407	CD	ARG B	106	9.631	20.446 20.546	20.746 21.842	1.00	50.57
	2408	NE	ARG B	106	10.970	20.223	21.346	1.00 1.00	51.15 50.88
35	2409	CZ	ARG B	106	12.013	19.938	22.120	1.00	42.48
	2410	NH1	ARG B	106	11.875	19.937	23.436	1.00	52.91
	2411	NH2	ARG B	106	13.191	19.650	21.581	1.00	40.82
	2412	C	ARG B	106	5.913	19.143	20.289	1.00	37.36
40	2413 2414	0 N	ARG B CYS B	106 107	5.488 6.304	18.406	21.199	1.00	26.46
10	2415	CA	CYS B	107	6.250	18.660 17.231	19.113 18.860	1.00	28.15
	2416	Ċ`	CYS B	107	7.669	16.735	18.872	1.00 1.00	29.34 42.87
	2417	0	CYS B	107	8.280	16.584	17.812	1.00	35.58
	2418	CB	CYS B	107	5.617	16.945	17.502	1.00	38.81
45	2419	SG	CYS B	107	5.072	15.220	17.305	1.00	55.53
	2420	N	HIS B	108	8.173	16.481	20.081	1.00	42.37
	2421 2422	CA CB	HIS B HIS B	108 108	9.544	16.022	20.296	1.00	43.07
	2423	CG	HIS B	108	9.947 11.374	16.267 15.931	21.751	1.00	59.40
50	2424	CD2	HIS B	108	11.925	15.232	22.052 23.068	1.00 1.00	55.40 55.98
	2425	ND1	HIS B	108	12.421	16.349	21.259	1.00	54.99
	2426	CE1	HIS B	108	13.558	15.919	21.776	1.00	62.39
	2427	NE2	HIS B	108	13.286	15.239	22.874	1.00	62.88
55	2428	C	HIS B	108	9.739	14.563	19.946	1.00	36.76
<i>33</i>	2429 2430	0	HIS B	108	9.008	13.698	20.440	1.00	16.46
	2431	N CA	GLY B GLY B	109	10.733	14.307	19.097	1.00	27.59
	2432	c ·	GLY B	109 109	11.001 12.066	12.953 12.233	18.656 19.446	1.00	39.81
	2433	ŏ	GLY B	109	13.025	12.841	19.903	1.00 1.00	36.02 45.53
60	2434	N	TRP B	110	11.902	10.925	19.589	1.00	45.09
	2435	CA	TRP B	110	12.842	10.094	20.328	1.00	42.50
	2436	CB	TRP B	110	12.456	8.614	20.147	1.00	42.85
	2437	CG	TRP B	110	13.388	7.739	20.893	1.00	47.55
65	2438	CD2	TRP B	110	13,360	7.449	22.295	1.00	54.18
J	2439 2440	CE2 CE3	TRP B	110	14.455	6.601	22.586	1.00	43.50
	2441	CD1	TRP B TRP B	110 110	12.518 14.459	7.855 7.0 5 6	23.339	1.00	57.45
	2442	NE1	TRP B	110	15.108	7.056 6.357	20.399 21.409	1.00	51.38
	2443	CZ2	TRP B	110	14.729	6.151	23.872	1.00 1.00	48.13 33.15
70	2444	CZ3	TRP B	110	12.793	7.403	24.629	1.00	55.46
				•		= =			····

	0445	2112							
	2445 2446	CH2 C	TRP B	110	13.894	6.557	24.877	1.00	49.35
	2447	ŏ.	TRP B	110 110	14.276 14.544	10.354 10.511	19.886 18.690	1.00	45.65
	2448	Ň	ARG B	111	15.182	10.388	20.866	1.00 1.00	34.73
5	2449	CA	ARG B	111	16.604	10.644	20.631	1.00	55.00 60.99
	2450	CB	ARG B	111	17.254	9.438	19.949	1.00	56.42
	2451	CG	ARG B	111	17.586	8.319	20.926	1.00	78.50
	2452	CD	ARG B	111	18.140	7.100	20.224	1.00	104.44
10	2453 2454	NE CZ	ARG B	111	18.757	6.157	21.154	1.00	117.08
10	2455	NH1	ARG B ARG B	111 111	19.996 20.766	6.272 7.291	21.628	1.00	124.78
	2456	NH2	ARG B	111	20.760	5.363	21.261 22.473	1.00 1.00	125.05
	2457	C	ARG B	111	16.813	11.896	19.790	1.00	126.10 67.62
	2458	0	ARG B	111	17.751	11.974	19.000	1.00	74.03
15	2459	N	ASN B	112	15.934	12.876	19.978	1.00	69.44
	2460	CA	ASN B	112	16.039	14.116	19.228	1.00	76,51
	2461 2462	CB CG	ASN B ASN B	112 112	17.207 17.150	14.964	19.725	1.00	84.90
	2463	OD1	ASN B	112	16.253	16.373 16.734	19.160 18.385	1.00	106.45
20	2464	ND2	ASN B	112	18.134	17.183	19.546	1.00 1.00	105.76 117.72
	2465	С	ASN B	112	16.155	13.785	17.751	1.00	79.76
	2466	0	ASN B	112	16.695	14.568	16.973	1.00	88.06
	2467	N	TRP B	113	15.686	12.614	17.372	1.00	76.72
25	2468 2469	CA CB	TRP B TRP B	113	15.721	12.245	15.953	1.00	59.95
20	2470	CG	TRP B	113 113	15.222 16.236	10.811 9.821	15.765	1.00	54.79
	2471	CD2	TRP B	113	16.046	8.442	16.180 16.5 2 3	1.00 1.00	40.29
	2472	CE2	TRP B	113	17.312	7.914	16.846	1.00	18.18 22.19
20	2473	CE3	TRP B	113	14.930	7.603	16.587	1.00	12.77
30	2474	CD1	TRP B	113	17.574	10.060	16.308	1.00	42.86
	2475 2476	NÉ1 CZ2	TRP 8	113	18.226	8.922	. 16.707	1.00	25.08
	2477	CZ2 CZ3	TRP B	113 113	17.493 15.111	6.587 6.286	17.228	1.00	22.94
	2478	CH2	TRP B	113	16.383	5.790	16.966 17.281	1.00 1.00	28.48
35	2479	C	TRP B	113	14.836	13.224	15.194	1.00	24.73 65.32
	2480	0	TRP B	113	13.936	13.822	15.777	1.00	68.76
	2481	N	ASP B	114	15.057	13.403	13.912	1.00	50.94
	2482 2483	CA CB	ASP B ASP B	114	14.164	14.252	13.145	1.00	52.09
40	2484	CG	ASP B ASP B	114 114	14.767 16.039	14.536 15.346	11.768	1.00	52.20
• •	2485	OD1	ASP B	114	16.065	16.368	11.830 12.546	1.00 1.00	66.27 80.90
	2486	OD2	ASP B	114	17.011	14.967	11.147	1.00	65.81
	2487	Č	ASP B	114	12.798	13.615	13.004	1.00	54.32
45	2488	0	ASP B	114	12.676	12.397	13.005	1.00	49.44
45	2489 2490	N CA	VAL B VAL B	115	11.762	14.429	12.886	1.00	59.6 5
	2491	CB	VAL B VAL B	115 115	10.408 9.542	13.936 14.291	12.713	1.00	44.63
	2492	CG1	VAL B	115	8.162	13.697	13.899 13.715	1.00 1.00	43.22
~^	2493	CG2	VAL B	115	10.192	13.802	15.156	1.00	33.45 33.33
50	2494	Ç	VAL B	115	9.876	14.672	11.497	1.00	60.55
	2495	0	VAL B	115	10.254	15.827	11.261	1.00	71.83
	2496 2497	N CA	TYR B	116	9.023	14.021	10.715	1.00	48.40
	2498	CA CB	TYR B TYR B	116 116	8.490 9.214	14.684 14.204	9.543	1.00	29.55
55	2499	ča	TYR B	116	10.708	14.436	8.299 8.299	1.00 1.00	25.24
	2500	CD1	TYR B	116	11.582	13.475	8.783	1.00	28.14 40.15
	2501	CE1	TYR B	116	12.956	13.645	8.691	1.00	52.64
	2502	CD2	TYR B	116	11.250	15.590	7.745	1.00	41.11
60	2503 2504	CE2	TYR B	116	12.635	15.770	7.651	1.00	48.69
00	2505	CZ OH	TYR B TYR B	116	13.478	14.797	8.127	1.00	44.88
	2506	C	TYR B	116 116	14.841 6.991	14.957 14.501	8.017 9.377	1.00 1.00	54.67
	2507	ŏ	TYR B	116	6.383	13.681	9.377 10.051	1.00	27.78 28.35
CF	2508	N	LYS B	117	6.409	15.265	8.460	1.00	26.33 38.88
65	2509	CA	LYS B	117	4.976	15.213	8.227	1.00	37.83
	2510 2511	CB	LYS B	117	4.567	13.922	7.508	1.00	47.24
	2511 2512	CD	LYS B Lys b	117	4.732	13.956	5.998	1.00	69.83
	2513	CE	LYS B	117 117	4.053 2.549	12.743 12.716	5.350 5.644	1.00	93.57
70	2514	NZ	LYS B	117	1.865	11.498	5.644 5.113	1.00 1.00	101.93
			_	• • •			0.110	1.00	91.83

	2515 2516	C	LYS B LYS B	117	4.347	15.264	9.603	1.00	25.37
	2517	N	VAL B	117 118	3.695	14.319	10.041	1.00	28.98
	2518	ČA	VAL B	118	4.568 4.014	16.374 16.513	10.296	1.00	23.24
5	2519	CB	VAL B	118	4.919	17.367	11.629 12.545	1.00	23.69
	2520	CG1	VAL B	118	4.205	17.627	13.868	1.00 1.00	38.59
	2521	CG2	VAL B	118	6.254	16.648	12.795	1.00	45.19 18.15
	2522	Ç	VAL B	118	2.650	17.152	11.593	1.00	18.84
10	2523 2524	0	VAL B	118	2.462	18.227	11.006	1.00	8.55
10	2524 2525	N CA	ILE B	119 119	1.700	16.503	12.250	1.00	12.98
	2526	CB	ILE B	119	0.355 -0.627	17.026 16.130	12.293	1.00	30.22
	2527	CG2	ILE B	119	-2.064	16.621	11.498 11.688	1.00 1.00	46.31
	2528	CG1	ILE B	119	-0.236	16.112	10.019	1.00	42.76 21.93
15	2529	CD1	ILE B	119	-1.236	15.436	9.133	1.00	51.60
	2530	C	ILE B	119	-0.076	17.038	13.734	1.00	38.62
	2531 2532	0 N	ILE B TYR B	119	0.261	16.123	14.483	1.00	47.55
	2533	CA	TYR B	120 120	-0.818 -1.312	18.068	14.125	1.00	32.69
20	2534	CB	TYR B	120	-0.950	18.148 19.474	15.489 16.123	1.00 1.00	32.47
	2535	CG	TYR B	120	0.503	19.596	16.455	1.00	16.42 25.56
	2536	CD1	TYR B	120	1.419	20.056	15.515	1.00	35.91
	2537	CE1	TYR B	120	2.771	20.205	15.844	1.00	51.47
25	2538 2539	CD2 CE2	TYR B	120	0.966	19.275	17.728	1.00	32.05
23	2540	CZ	TYR B TYR B	120 120	2.311 3.209	19.412	18.070	1.00	29.56
	2541	OH	TYR B	120	4.537	19.883 20.063	17.123 17.438	1.00	44.13
	2542	C	TYR B	120	-2.806	18.001	15.490	1.00 1.00	29.40 33.00
	2543	0	TYR B	120	-3.484	18.535	14.625	1.00	54.53
30	2544	N	TYR B	121	-3.322	17.277	16.467	1.00	31.54
	2545 2546	CA	TYR B	121	-4.744	17.066	16.544	1.00	38.10
	2546 2547	CB CG	TYR B TYR B	121 121	-5.068	15.570	16.402	1.00	34.72
	2548	CD1	TYR B	121	-4. 63 5 -3.293	14.953 14.656	15.087 14.855	1.00	45.90
35	2549	CE1	TYR B	121	-2.878	14.083	13.654	1.00 1.00	43.35 44.63
	2550	CD2	TYR B	121	-5.570	14.659	14.076	1.00	45.04
	2551	CE2	TYR B	121	-5. 169	14.078	12.874	1.00	37.76
	2552 2553	CZ OH	TYR B	121	-3.822	13.796	12.675	1.00	47.75
40	2554	C	TYR B TYR B	121 121	-3.411 -5.272	13.225	11.502	1.00	43.41
	2555	ŏ	TYR B	121	-4.735	17.579 17.246	17.864 18.927	1.00 1.00	51.86
	2556	N	LYS B	122	-6.314	18.403	17.794	1.00	65.44 51.19
	2557	CA	LYS B	122	-6.957	18.914	18.992	1.00	60.52
45	2558	CB	LYS B	122	-7.037	20.435	18.969	1.00	58.03
43	2559 2560	CG CD	LYS B LYS B	122	-7.268	21.024	20.357	1.00	76.69
	2561	CE	LYS B	122 122	-7.727 -9.203	22.472 22.561	20.312	1.00	76.94
	2562	NZ	LYS B	122	-9.694	23.961	19.973 20.057	1.00 1.00	78.85
	2563	C	LYS B	122	-8.368	18.331	19.016	1.00	78.17 69.22
50	2564	0	LYS B	122	-9.259	18.817	18.314	1.00	71.75
	2565	N	ASP B	123	-8.554	17.283	19.814	1.00	75.25
	2566 2567	CA	ASP B	123	-9.840 10.050	16.611	19.936	1.00	81.83
	2568	CG	ASP B	123 123	-10.952 -10.809	17.623	20.242	1.00	85.33
55	2569	OD1	ASP B	123	-10.750	18.253 17.499	21.618 22.613	1.00 1.00	86.97
	2570	OD2	ASP B	123	-10.764	19.501	21.703	1.00	97.59 80.57
	2571	C	ASP B	:23	-10.172	15.841	18.660	1.00	85.87
	2572	0	ASP B	123	-11.183	16.107	18.002	1.00	90.87
60	2573 2574	N CA	GLY B GLY B	124	-9.310	14.889	18.314	1.00	83.44
00	2575	Ĉ	GLY B	124 124	-9.538 -0.393	14.080	17.131	1.00	83.47
	2576	ŏ	GLY B	124	-9.383 -9.053	14.835 14.236	15.826 14.804	1.00 1.00	82.06 80.62
	2577	Ñ	GLU B	125	-9.615	16.144	15.847	1.00	80.62 76.60
<i>C</i> F	2578	ÇA	GLU B	125	-9.479	16.951	14.640	1.00	69.95
65	2579	CB	GLU B	125	-10.431	18.146	14.697	1.00	83.15
	2580 2581	CG CD	GLU B	125	-11.903	17.778	14.854	1.00	99.12
	2582	CD OE1	GLU B GLU B	125 125	-12.808 -12.297	19.009	14.961	1.00	110.18
	2583	OE2	GLU B	125	-12.287 -14.041	20.153 18.828	14.909	1.00	115.12
70	2584	C	GLU B	125	-8.043	17.452	15.099 14.501	1.00 1.00	112.68 59.20
								1.50	33.20

	2585	0	GLU B	125	-7.370	17.681	15.493	1.00	60 00
	2586	N	ALA B	126	-7.574	17.609	13.269	1.00	68.90 55.84
	2587 2588	CA CB	ALA B ALA B	126	-6.221	18.112	13.032	1.00	49.26
5	2589	C	ALA B	126 126	-5.783 -6.229	17.788 19.623	11.636	1.00	37.55
•	2590	ŏ	ALA B	126	-7.288	20.251	13. <u>22</u> 9 13.192	1.00	55.35
	2591	N	LEU B	127	-5.053	20.211	13.425	1.00 1.00	62.37
	2592	CA	LEU B	127	-4.968	21.648	13.652	1.00	58.36 56.69
10	2593 2594	CB	LEU B	127	-4.821	21.938	15.148	1.00	64.48
10	259 4 2595	CG CD1	LEU B LEU B	127 127	-4. 60 6 -5.705	23.411	15.496	1.00	71.37
	2596	CD2	LEU B	127	-5.705 -4.590	24.262 23.573	14.864 17.012	1.00	76.49
	2597	С	LEU B	127	-3.837	22.314	12.895	1.00 1.00	74.87 59.25
15	2598	0	LEV B	127	-3.979	23.463	12.449	1.00	65.52
15	2599 2600	N CA	LYS B	128	-2.710	21.619	12.760	1.00	39.64
	2601	CA CB	LYS B LYS B	128	-1.583	22.176	12.022	1.00	49.21
	2602	CG	LYS B	128 128	-0.695 -1.370	23.067 24.362	12.911	1.00	55.50
	2603	CD	LYS B	128	-0.363	25.479	13.365 13.615	1.00 1.00	77.67
20	2604	CE	LYS B	128	-1.085	26.778	13.981	1.00	85.20 95.26
	2605	NZ	LYS B	128	-0.159	27.945	14.093	1.00	94.69
	2606 2607	C	LYS B	128	-0.743	21.091	11.397	1.00	47.41
	2608	0 N	LYS B TYR B	128	-0.639	19.967	11.917	1.00	56.27
25	2609	CA	TYR B	129 129	-0.181 0.682	21.412 20.491	10.277	1.00	25.40
	2610	CB	TYR B	129	-0.094	19.800	9.551 8.429	1.00	31.17
	2611	CG	TYR B	129	0.773	18.963	7.516	1.00 1.00	9.94 7.68
	2612	CD1	TYR B	129	0.995	17.618	7.780	1.00	13.54
30	2613	CE1	TYR B	129	1.788	16.850	6.948	1.00	15.62
30	2614 2615	CD2 CE2	TYR B	129	1.370	19.519	6.393	1.00	9.74
	2616	CZ	TYR B TYR B	129 129	2.164 2.369	18.759	5.558	1.00	6.56
	2617	OH	TYR B	129	3.160	17.425 16.667	5.839 5.007	1.00	23.46
	2618	C	TYR B	129	1.905	21.203	8.987	1.00 1.00	29.69 18.84
35	2619	0	TYR B	129	1.810	22.418	8.723	1.00	20.48
	2620	N	TRP B	130	2.983	20.508	8.856	1.00	10.01
	2621 2622	CA CB	TRP B	130	4.195	21.121	8.376	1.00	26.80
	2623	CG	TRP B	130 130	4.621 5.657	22.248 23.141	9.331	1.00	24.97
40	2624	CD2	TRP B	130	5.463	24.474	8.763 8.258	1.00 1.00	34.86
	2625	CE2	TRP B	130	6.718	24.933	7.789	1.00	19.75 18.96
	2626	CE3	TRP B	130	4.338	25.321	8.160	1.00	4.59
	2627	CD1	TRP B	130	6.995	22.854	8.577	1.00	46.79
45	2628 2629	NE1 CZ2	TRP B	130	7.637	23.935	7.990	1.00	33.27
	2630	CZ3	TRP B	130 130	6.887 4.513	26.195 26,582	7.230	1.00	7.20
	2631	CH2	TSP B	130	5.778	27.003	7.599 7.141	1.00 1.00	26.73
	2632	С	TRP B	130	5.204	19.990	8.359	1.00	33.91 28.67
50	2633	0	TRP B	130	5.511	19.385	9.388	1.00	37.85
30	2634 2635	N CA	TYR B	131	5.686	19.697	7.164	1.00	25.88
	2636	CB	TYR B TYR B	131 131	6.639 7.327	18.631	6.919	1.00	25.53
	2637	CG	TYR B	131	7.327 8.003	18.864	5.599	1.00	12.69
	2638	CD1	TYR B	131	7.258	17.638 16.534	5.076 4.672	1.00 1.00	27.25
55	2639	CE1	TYR B	131	7.893	15.406	4.143	1.00	27.89 37.49
	2640	CD2	TYR B	131	9.385	17.589	4.949	1.00	47.62
	2641 2642	CE2	TYR B	131	10.030	16.477	4.424	1.00	47.79
	2643	CZ OH	TYR B TYR B	131	9.287	15.394	4.023	1.00	46.72
60	2644	Č.	TYR B	131 131	9.948 7.699	14.315 18.490	3.487	1.00	44.87
	2645	Õ	TYR B	131	7.730	17.491	7.988 8.714	1.00 1.00	41.53
	2646	N	GLU B	132	8.584	19.481	8.058	1.00	45.44 41.35
	2647	CA	GLU B	132	9.651	19.477	9.045	1.00	23.47
65	2648 2649	CB CC	GLU B	132	10.631	20.595	8.746	1.00	26.69
0 ,5	2649 2650	CD	GLU B GLU B	132	11.512	20.343	7.517	1.00	30.91
	2651	OE1	GLU B	132 132	12.674 12.695	19.419	7.819	1.00	59.01
	2652	OE2	GLU B	132	13.555	18.835 19.276	8.933 6.939	1.00	78.14 45.20
70	2653	C	GLU B	132	9.017	19.678	10.410	1.00 1.00	45.30 30.80
70	2654	0	GLU B	132	7.926	20.252	10.503	1.00	15.18
				•				-	. 31.14

	2655 2656 2657	N CA CB :	ASN B ASN B ASN B	133 133 133	9.673 9.078 9.969	19.198 19.340	11.466 12.785	1.00	38.68 35.69
5 ,	2658 2659 2660	CG OD1 ND2	ASN B ASN B ASN B	133 133 133	9.165 8.183 9.582	18.765 18.350 19.018 17.243	13.884 15.126 15.524 15.745	1.00 1.00 1.00	24.76 52.21 35.03
	2661 2662 2663	C O N	ASN B ASN B HIS B	133 133 134	8.857 9.651 7.770	20.813 21.644 21.132	13.030 12.587 13.718	1.00 1.00 1.00 1.00	43.95 29.20 43.35
10	2664 2665 2666	CA CB CG	HIS B HIS B HIS B	134 134 134	7.435 6.522 5.268	22.506 23.054 22.256	14.022 12.927 12.734	1.00 1.00 1.00	15.66 21.19 41.57 45.84
15	2667 2668 2669	CD2 ND1 CE1	HIS B HIS B	134 134 134	3.972 5.280 4.037	22.543 20.969 20.507	12.990 12.228 12.183	1.00 1.00 1.00	30.22 29.02 45.78
	2670 2671 2672 2673	NE2 C O N	HIS B HIS B	134 134 134	3.230 6.733 6.072	21.443 22.587 21.631	12.640 15.380 15.826	1.00 1.00 1.00	39.55 30.10 22.57
20	2674 2675 2676	CA CB CG	ASN B ASN B ASN B	135 135 135 135	6.871 6.263 7.182	23.731 23.933 24.741	16.043 17.355 18.303	1.00 1.00 1.00	35.59 43.05 49.56
25	2677 2678 2679	OD1 ND2 C	ASN B ASN B ASN B	135 135 135 135	8.585 8.717 9.614 5.006	24.138 22.936 24.991 24.761	18.481 18.749 18.356	1.00 1.00 1.00	62.83 59.97 50.35
	2680 2681 2682	O N CA	ASN B ILE B ILE B	135 136 136	5.024 3.910 2.720	25.700 24.406 25.244	17.162 16.384 17.820 17.749	1.00 1.00 1.00 1.00	31.65 53.46 39.40
30	2683 2684 2685	CB CG2 CG1	ILE B ILE B ILE B	136 136 136	1.440 0.254 1.232	24.484 25.448 23.368	18.081 18.105 17.065	1.00 1.00 1.00	46.75 51.16 27.02 48.68
25	2686 2687 2688	CD1 C O	ILE B ILE B ILE B	136 136 136	-0.057 2.922 2.996	22.599 26.304 25.995	17.259 18.834 20.026	1.00 1.00 1.00	57.62 57.38 38.50
35	2689 2690 2691 2692	N CA CB	SER B SER B	137 137 137	3.035 3.238 4.495	27.554 28.653 29.443	18.409 19.333 18.941	1.00 1.00 1.00	62.66 62.59 62.06
40	2693 2694 2695	OG C O N	SER B SER B SER B ILE B	137 137 137	4.789 2.015 1.675	30.448 29.557 30.140	19.899 19.314 18.295	1.00 1.00 1.00	70.77 54.31 61.87
	2696 2697 2698	CA CB CG2	ILE B ILE B ILE B	138 138 138 138	1.344 0.167 •1.060 •2.289	29.665 30.511 29.702 30.588	20.450 20.551 20.970	1.00 1.00 1.00	57.19 64.51 66.59
45	2699 2700 2701	CG1 CD1 C	ILE B ILE B ILE 5	138 138 138	-1.244 -2.439 0.409	28.528 27.657 31.600	20.965 20.011 20.338 21.581	1.00 1.00 1.00 1.00	62.45 72.23 72.19 70.00
50	2702 2703 2704	O N CA	ILE B THR B THR B	138 139 139	0.207 0.846 1.143	31.396 32.760 33.914	22.777 21.100 21.951	1.00 1.00 1.00	80.22 75.14 76.04
	2705 2706 2707 2708	CB OG1 CG2 C	THR B THR B THR B THR B	139 139 139	1.419 0.347 2.720	35.149 35.322 34.969	21.086 20.153 20.312	1.00 1.00 1.00	66.84 70.10 62.07
55	2709 2710 2711	O N CA	THR B ASN B ASN R	139 139 140 140	0.064 0.333 -1.142 -2.244	34.246 34.206 34.598 34.893	22.993 24.190 22.553	1.00 1.00 1.00	77.29 88.78 78.71
60	2712 2713 2714	CB CG OD1	ASN B ASN B ASN B	140 140 140	-2.994 -2.195 -2.591	36.169 37.465 38.486	23.485 23.082 23.304 22.747	1.00 1.00 1.00 1.00	86.24 96.34 113.86 123.78
	2715 2716 2717	ND2 C O	ASN B ASN B ASN B	140 140 140	-1.120 -3.245 -3.962	37.473 33.716 33.521	24.100 23.456 22.474	1.00 1.00 1.00	121.56 84.41 92.35
65	2718 2719 2720	N CA CB	ALA B ALA B ALA B	141 141 141	-3.298 -4.186 -3.768	32.944 31.781 30.931	24.536 24.642 25.819	1.00 1.00 1.00	74.85 70.00 60.72
70	2721 2722 2723 2724	C O N CA	ALA B ALA B THR B THR B	141 141 142	-5.679 -6.083 -6.486	32.080 33.215 31.033	24.744 25.000 24.557	1.00 1.00 1.00	73.54 71.12 79.19
	7	<u> </u>	INN D	142	-7.945	31.135	24.602	1.00	81.65

	2725	CB	THR B	142	-8.550	31.294	23.191	1.00	87.55
	2726	OG1	THR B	142	-7.856	32.324	22.475	1.00	87.31
	2727 2728	CG2.	THR B	142	-10.032	31.647	23.292	1.00	80.50
5	2729	C	THR B THR B	142	-8.556	29.872	25.196	1.00	81.42
-	2730	Ň	VAL B	142 143	-8.001 -9.716	28.782 30.022	25.063	1.00	80.47
	2731	ĈA	VAL B	143	-10.385	28.881	25.828 26.436	1.00	79.19
	2732	СВ	VAL B	143	-11.681	29.314	27.154	1.00 1.00	80.64 85.23
10	2733	CG1	VAL B	143	-12.667	29.899	26.146	1.00	91.61
10	2734	CG2	VAL B	143	-12.293	28.123	27.880	1.00	91.42
	2735 2736	C	VAL B VAL B	143	-10.728	27.848	25.370	1.00	78.44
	2737	Ň	GLU B	143 144	-10.878	26.659	25.659	1.00	67.92
	2738	ČA	GLU B	144	-10.847 -11.173	28.317 27.438	24.132 23.019	1.00	87.88
15	2739	CB	GLU B	144	-11.546	28.261	21.775	1.00 1.00	94.42 103.89
	2740	CG	GLU B	144	-12.116	27.439	20.605	1.00	127.47
	2741	CD	GLU B	144	-13.460	26.781	20.925	1.00	145.47
	2742 2743	OE1	GLU B	144	-14.018	27.052	22.011	1.00	154.66
20	2743	OE2 C	GLU B GLU B	144 144	-13.960	25.995	20.087	1.00	153.18
20	2745	ŏ	GLU B	144	-9.977 -10.137	26. 54 6 25. 38 5	22.721	1.00	87.49
	2746	Ň	ASP B	145	-8.777	27.086	22.328 22.919	1.00 1.00	92.98 73.99
	2747	CA	ASP B	145	-7.557	26.336	22.674	1.00	73.40
25	2748	CB	ASP B	145	-6.348	27.253	22.815	1.00	76.84
25	2749 2750	CG	ASP B	145	-6.159	28.159	21.614	1.00	84.39
	2750 2751	OD1 OD2	ASP B ASP B	145 145	-6.061	27.632	20.481	1.00	89.54
	2752	C	ASP B	145	-6.101 -7.434	29.394 25.135	21.801	1.00	78.78
	2753	Ö	ASP B	145	-6.468	24.371	23.618 23.546	1.00 1.00	72.65
30	2754	N	SER B	146	-8.423	24.971	24.496	1.00	66.12 68.40
	2755	CA	SER B	146	-B.445	23.857	25.441	1.00	59.96
	2756	CB	SER B	146	-9.433	24.128	26.579	1.00	59.40
	2757 2 7 58	OG C	SER B SER B	146	-8.959	25.158	27.435	1.00	82.76
35	2759	ŏ	SER B	146 146	-8.862 -9.531	22.590 22.649	24.725	1.00	55.02
	2760	Ň	GLY B	147	-8.462	21.447	23.703 25.267	1.00 1.00	74.05 55.86
	2761	CA	GLY B	147	-8.811	20.174	24.662	1.00	55.22
	2762	Č	GLY B	147	-7.680	19.168	24.739	1.00	55.94
40	2763 2764	0	GLY B	147	-6.624	19.453	25.308	1.00	65.07
70	2765	N CA	THR B THR B	148 148	-7.895 -6.871	17.984	24.173	1.00	51.77
	2766	CB	THR B	148	-7.493	16.945 15.537	24.186 24.299	1.00 1.00	56.97
	2767	OG1	THR B	148	-7.822	15.054	22.992	1.00	62.53 93,22
45	2768	CG2	THR B	148	-8.769	15.581	25.130	1.00	61.98
45	2769	C	THR B	148	-6.061	17.028	22.895	1.00	50.21
	2770 2771	O N	THR B TYR B	148	-6.605	16.990	21.803	1.00	61.31
	2772	ČA	TYR B	149 149	-4.752 -3.873	17.167 17 .26 3	23.026	1.00	47.96
	2773	CB	TYR B	149	-2.907	18.438	21.870 22.008	1.00 1.00	36.15
50	2774	CG	TYR B	149	-3.504	19.814	21.873	1.00	39.15 32.57
	2775	CD1	TYR B	149	-4.170	20.418	22.932	1.00	43.98
	2776	CE1	TYR B	149	-4.695	21.704	22.815	1.00	43.58
	2777 2778	CD2 CE2	TYR B	149	-3.382	20.525	20.687	1.00	33.74
55	2779	CZ	TYR B TYR B	149 149	-3.909 -4.564	21.810 22.396	20.553	1.00	35.76
	2780	OH OH	TYR B	149	-5.089	23.668	21.621 21.494	1.00 1.00	41.82 40.18
	2781	С	TYR B	149	-3.028	16.013	21.730	1.00	38.28
	2782	0	TYP B	149	-2.944	15.191	22.651	1.00	37.42
60	2783	N	TYR B	150	-2.386	15.893	20.573	1.00	28.35
00	2784 2785	CA CB	TYR B	150	-1.500	14.776	20.287	1.00	32.70
	2786	CG	TYR B TYR B	150 150	-2.226 -3.180	13.421	20.440	1.00	46.79
	2787	CD1	TYR B	150	-3.180 -2.710	13.018 12.397	19.328 18.168	1.00 1.00	40.91 38.70
	2788	CE1	TYR B	150	-3.588	12.007	17.150	1.00	38.70 49.78
65	2789	CD2	TYR B	150	-4.556	13.245	19.447	1.00	29.49
	2790	CE2	TYR B	150	-5.440	12.862	18.436	1.00	54.83
	2791 2792	CZ OH	TYR B	150	-4.950 5.000	12.245	17.294	1.00	51.46
	2793	C	TYR B TYR B	150 150	-5.828 -1.002	11.857	16.310	1.00	68.38
70	2794	ŏ	TYR B	150	-1.002 -1.718	14.971 15.477	18.880 18.028	1.00 1.00	30.40
					10			1.00	49.73

	2795 2796	N CA	CYS B	151 151	0.241 0.808	14.596 14.746	18.645	1.00	25.26
	2797	č	CYS B	151	1.175	13.410	17.326 16.699	1.00	39.72
_	2798	Ō	CYS B	151	1.270	12.395	17.383	1.00 1.00	37.05
5	2799	CB	CYS B	151	2.040	15.652	17.399	1.00	49.88 44.87
	2800	SG	CYS B	151	3.415	15.099	18.482	1.00	47.69
	2801 2802	N	THR B	152	1.380	13.419	15.387	1.00	34.36
	2803	CA CB	THR B	152	1.753	13 217	14.648	1.00	40.90
10	2804	OG1	THR B	152 152	0.641 0.435	11.715 12.666	13.712	1.00	46.04
	2805	CG2	THR B	152	-0.652	11.514	12.656 14.487	1.00	59.44
	2806	· C	THR B	152	2.906	12.646	13.784	1.00 1.00	54.68
	2807	0	THR B	152	3.063	13.845	13.500	1.00	39.86 42.60
15	2808	N	GLY B	153	3.707	11.680	13.355	1.00	28.17
15	2809	CA	GLY B	153	4.846	12.024	40 نا2.	1.00	26.12
	2810 2811	C	GLY B GLY B	153 153	5.647	10.818	12,112	1.00	33.14
	2812	Ň	LYS B	154	5.622 6.365	9.753 10.998	12.734	1.00	34.08
	2813	ĈA	LYS B	154	7.188	9.959	11.021 10.471	1.00 1.00	17.31
20	2814	CB	LYS B	154	7.185	12.086	8.949	1.00	31.41 56.81
	2815	CG	LYS B	154	8.472	9.571	8.248	1.00	78.50
	2816	CD	LYS B	154	8.399	10.064	6.771	1.00	85.12
	2817 2818	CE	LYS B	154	9.733	9.881	6.064	1.00	88.41
25	2819	NZ C	LYS B LYS B	154	9.649	10.343	4.653	1.00	64.75
	2820	ŏ	LYS B	154 154	8.597 9.266	10. 101 11.116	11.028	1.00	44.08
	2821	Ň	VAL B	155	9.027	9.078	10.811 11.762	1.00 1.00	51.89
	2822	CA	VAL B	155	10.362	9.047	12.345	1.00	46.05 43.86
20	2823	CB	VAL B	155	10.321	8.903	13.878	1.00	37.35
30	2824	CG1	VAL B	155	11.732	8.926	14.416	1.00	21.63
	2825 2826	CG2	VAL B	155	9.487	10.030	14.499	1.00	48.98
	2827	C O	VAL B VAL B	155 155	11.035 10.560	7.823	11.779	1.00	41.23
	2828	Ň	TRP B	156	12.129	6.716 8.012	11.989 11.057	1.00	37.63
35	2829	CA	TRP B	156	12.824	6.880	10.454	1.00 1.00	52.20 74.29
	2830	CB	TRP B	156	13.196	5.838	11.510	1.00	65.13
	2831	CG	TRP B	156	14.467	6.147	12.211	1.00	70.49
	2832 2833	CD2	TRP B	156	15.771	6.221	11.629	1.00	54.80
40	2834	CE2 CE3	TRP B	156	16.670	6.585	12.646	1.00	64.98
	2835	CD1	TRP B	156 156	16.252 14.631	6.012 6.458	10.334 13.539	1.00	50.71
	2836	NE1	TRP B	156	15.954	6.725	13.804	1.00 1.00	71.39 63.30
	2837	CZ2	TRP B	156	18.051	6.752	12.415	1.00	62.21
45	2838	CZ3	TRP B	156	17.624	6.179	10.101	1.00	67.16
45	2839 2840	CH2	TRP B	156	18.500	6.545	11.141	1.00	53.68
	2840 2841	C O	TRP B TRP B	156	12.015	6.201	9.347	1.00	90.81
	2842	Ň	GLN B	156 157	11.962 11.389	4.971 7.013	9.263	1.00	111.59
	2843	ĊA	GLN B	157	10.608	6.526	8.506 7.382	1.00 1.00	88.48
50	2844	СВ	GLN B	157	11.461	5.575	6.536	1.00	85.04 110.53
	2845	CG	GLN B	157	10.930	5.324	5.138	1.00	124.62
	2846	CD	GLN B	157	11.824	4.383	4.337	1.00	129.56
	2847 2848	OE1	GLN B	157	12.951	4.080	4.749	1.00	127.90
55	2849	NE2 C	GLN B GLN B	157	11.329	3.926	3.183	1.00	123.80
-	2850	ŏ	GLN B	157 157	9.311 8.544	5.842 5.392	7.816	1.00	78.48
	2851	Ň	LEU B	158	9.074	5.760	6.977 • 9.122	1.00 1.00	77.35 70.67
	2852	CA	LEU B	158	7.849	5.147	9.635	1.00	70.67 70.41
۲۸	2853	CB	LEU B	158	8.170	4.049	10.637	1.00	81.95
60	2854	CG	LEU B	158	8.646	2.722	10.055	1.00	86.23
	2855 2856	CD1	LEU B	158	8.865	1.715	11.174	1.00	105.28
	2857	CD2 C	LEU B LEU B	158 158	7.602	2.204	9.081	1.00	94.27
	2858	ŏ	LEU B	158 158	6.998 7.499	6.203 7.275	10.313	1.00	70.44
65	2859	Ň	ASP B	159	7.489 5.721	7.275 5.904	10.632 10.537	1.00 1.00	80.05 67.41
	2860	CA	ASP B	159	4.837	6.880	11.171	1.00	82.00
	2861	CB	ASP B	159	3.519	7.001	10.392	1.00	86.28
	2862	CG	ASP B	159	3.736	7.375	8.938	1.00	106.10
70	2863 2864	OD1 OD2	ASP B	159	4.285	8.469	8.664	1.00	117.95
, ,		JUZ	ASP B	159	3.361	6.564	8.067	1.00	115.39

	2865	С	ASP B	159	4,547	6 405	10.014		
	2866	ŏ	ASP B	159	4.590	6.495 5.316	12.611 12.962	1.00	77.19
	2867	Ň	TYR B	160	4,274	7.492	13.448	1.00 1.00	77.19
_	2868	CA	TYR B	160	3.972	7.232	14.842	1.00	65.57
5	2869	CB	TYR B	160	5.244	7.273	15.670	1.00	48.77 37.12
	2870	CG	TYR B	160	6.332	6.371	15.148	1.00	34.46
	2871	CD1	TYR B	160	7.199	6.797	14.134	1.00	37.79
	2872	CE1	TYR B	160	8.195	5.961	13.645	1.00	56.87
10	2873	CD2	TYR B	160	6.490	5.086	15.661	1.00	19.69
10	2874	CE2	TYR B	160	7.486	4.233	15.179	1.00	40.99
	2875 2876	CZ OH	TYR B	160	8.341	4.674	14.172	1.00	60.40
	2877	C	TYR B TYR B	160 160	9.343 3.000	3.841	13.702	1.00	70.89
	2878	ŏ	TYR B	160	2.718	8.266 9.265	15.364	1.00	54.13
15	2879	Ň	GLU B	161	2.716	8.022	14.687	1.00	60.44
	2880	CA	GLU B	161	1.546	8.926	16.569 17.193	1.00	47.74
	2881	СВ	GLU B	161	0.133	8.387	16.988	1.00	48.57
	2882	CG	GLU B	161	-0.965	9.106	17.748	1.00	55.17 80.84
	2883	CD	GLU B	161	-2.360	8.757	17.226	1.00	93.70
20	2884	OE1	GLU B	161	-3.352	9.054	17.932	1.00	99.33
	2885	Ĵ E2	GLU B	161	-2.465	8.198	16.106	1.00	101.86
	2886	C	GLU B	161	1.872	9.038	18.671	1.00	56.41
	2887	0	GLU B	161	2.080	8.028	19.340	1.00	58.09
25	2888 2889	N CA	SER B	162	1.928	10.268	19.173	1.00	61.15
. 23	2890	CA CB	SER B SER B	162	2.240	10.515	20.578	1.00	70.01
	2891	OG	SER B	162 162	2.700	11.965	20.771	1.00	82.47
	2892	Č	SER B	162	1.646 1.046	12.889 10.258	20.523	1.00	75.43
	2893	ŏ	SER B	162	-0.083	10.163	21.481 21.017	1.00	69.94
30	2894	Ň	GLU B	163	1.301	10.133	22.776	1.00 1.00	70.40
	2895	CA	GLU B	163	0.223	9.924	23.728	1.00	76.24 74.01
	2896	CB	GLU B	163	0.785	9.585	25.106	1.00	83.42
	2897	CG	GLU B	163	1.437	8.222	25.201	1.00	108.95
25	2898	CD	GLU B	163	0.421	7.096	25.165	1.00	124.63
35	2899	OE1	GLU B	163	-0.463	7.070	26.051	1.00	126.10
	2900	OE2	GLU B	163	0.507	6.239	24.255	1.00	137.68
	2901 2902	C	GLU B	163	-0.517	11.246	23.809	1.00 \	64.66
	2903	N	GLU B PRO B	163 164	0.096	12.303	23.836	1.00	78.89
40	2904	CD	PRO B	164	-1.848 -2.763	11.211	23.829	1.00	49.91
	2905	CA	PRO B	164	-2.763	10.066 12.477	23.886 23.912	1.00	45.53
	2906	СВ	PRO B	164	-4.040	12.042	23.913	1.00 1.00	49.79 50.14
	2907	CG	PRO B	164	-3.988	10.692	24.532	1.00	54.43
	2908	С	PRO B	164	-2.210	13.229	25.177	1.00	52.68
45	2909	0	PRO B	164	-1.676	12.650	26.121	1.00	55.25
	2910	N	LEU B	165	-2.496	14.523	25.187	1.00	46.01
	2911	CA	LEU B	165	-2.195	15.363	26.330	1.00	38.63
	2912	CB	LEU B	165	-0.862	16.080	26.112	1.00	42.39
50	2913 2914	CG CD1	LEU B LEU B	165	-0.390	17.012	27.232	1.00	34.72
50	2915	CD2	LEU B LEU B	165 165	0.058	16.181	28.423	1.00	36.79
	2916	C	LEU B	165	0.765	17.879	26.732	1.00	31.18
	2917	ŏ	LEU B	165	-3.306 -3.561	16.390	26.491	1.00	41.11
	2918	Ñ	ASN 6	166	-3.983	17.181 16.369	25.597 27.626	1.00	47.00
55	2919	CA	ASN B	166	-5.044	17.332	27 352	1.00 1.00	47.91 62.56
	2920	CB	ASN B	166	-5.919	16.892	29.031	1.00	89.42
	2921	CG	ASN P	166	-6.897	15.795	28.644	1.00	111.40
	2922	OD1	ASN B	166	-7.511	15.874	27.581	1.00	117.56
60	2923	ND2	ASN B	166	-7.069	14.782	29.490	1.00	128.12
60	2924	C	ASN B	166	-4.419	18.685	28.139	1.00	63.19
	2925	0	ASN B	166	-3.385	18.758	28.798	1.00	75.62
	2926 2927	N CA	ILE B	167	-5.028	19.743	27.614	1.00	55.85
	2928	CA CB	ILE B ILE B	167	-4.547	21.103	27.837	1.00	50.63
65	2929	CG2	ILE B ILE B	167 167	-3.775 -3.644	21.642	26.625	1.00	41.65
	2930	CG1	ILE B	167	-3.644 -2.398	23.158	26.704	1.00	27.67
	2931	CD1	ILE B	167	-2.386 -1.576	20.981 21.401	26.572 25.373	1.00	49.69
	2932	C	ILE B	167	-5.719	22.018	25.373 28.127	1.00 1.00	71.73 52.51
=-	2933	Ō	ILE B	167	-6.636	22,141	27.328	1.00	52.51 54.25
70	2934	N	THR B	168	-5.677	22.669	29.279	1.00	62.54

PCT/US99/26203

	2935 2936	CA CB	THR B	168 168	-6.762 -7.371	23.552 23.090	29.872 30.995	1.00 1.00	73.12 77.82
	2937	OG1	THR B	168	·7.229	21.668	31.116	1.00	71.03
5	2938 2939	CG2 C	THR B	168	-8.847	23.472	31.049	1.00	80.41
,	2939	ŏ	THR B THR B	168	-6.329	25.002	29.841	1.00	79.24
	2941	Ň	VAL B	168 169	-5.347 7.070	25.294 25.907	30.526	1.00	81.73
	2942	CA	VAL B	169	-7.070 -6.792	25.907 27.336	29.214	1.00	81.68
	2943	CB	VAL B	169	-6.787	27.996	29.302	1.00	82.56
10	2944	CG1	VAL B	169	-6.538	29.487	27.916 28.048	1.00	80.42
	2945	CG2	VAL B	169	-5.731	27.352	27.041	1.00 1.00	71.55
	2946	C	VAL B	169	-7.937	27.908	30.115	1.00	82.46
	2947	0	VAL B	169	-9.098	27.841	29.696	1.00	89.49 87.82
	2948	N	ILE B	170	-7.625	28.469	31.277	1.00	94.48
15	2949	CA	ILE B	170	-8.668	28.995	32.143	1.00	101.94
	2950	СВ	ILE B	170	-8.332	28.730	33.631	1.00	98.82
	2951	CG2	ILE B	170	-8.574	27.262	33.966	1.00	99.33
	2952	CG1	ILE B	170	-6.876	29.092	33.912	1.00	103.85
20	2953 2954	CD1	ILE B	170	-6.453	28.836	35.347	1.00	102.26
20	295 4 2955	C O	ILE B	170	-9.027	30.467	31.967	1.00	106.09
	2956	NI	LYS B	170 171	-8.162	31.307	31.727	1.00	103.79
	2957	CA	LYS B	171	-10.326 -10.870	30.715 32.069	32.066	1.00	115.25
	2958	CB	LYS B	171	-12.374	32.030	32.000	1.00	116.92
25	2959	ČĞ	LYS B	171	-13.021	33.402	31.674 31.721	1.00	111.37
	2960	CD	LYS B	171	-12.523	34.293	30.594	1.00 1.00	106.02
	2961	CE	LYS B	171	-13.256	35.629	30.587	1.00	110.98
	2962	NZ	LYS B	171	-12.673	36.579	29.609	1.00	109.27 99.03
	2963	С	LYS B	171	-10.606	32.682	33.357	1.00	122.05
30	2964	0	LYS B	171	-10.455	31.952	34.327	1.00	122.45
	2965	N	ALA B	172	-10.550	34.004	33.492	1.00	121.93
	2966	CA	ALA B	172	-10.154	34.550	34.807	1.00	124.78
	2967	CB	ALA B	172	-8.778	35.182	34.669	1.00	110.24
35	2968	C	ALA B	172	-11.069	35.577	35.528	1.00	131.95
33	2969 2970	O N	ALA B	172	-11.006	36.782	35,303	1.00	136.47
	2971	CD	PRO B PRO B	173	-11.911	35.025	36.361	1.00	138.57
	2972	CA	PRO B	173 173	-12.775	34.002	35.754	1.00	133.76
	2973	CB	PRO B	173	-12.781 -13.714	35.842 34.799	37.272 37.970	1.00	145.56
40	2974	ČĠ	PRO B	173	-13.935	33.894	37.872 36.705	1.00	143.51
	2975	Č	PRO B	173	-12.008	36.690	38.273	1.00 1.00	139.83
	2976	0	PRO B	173	-10.896	36.332	38.614	1.00	152.09 158.41
	2977	N	ARG B	174	-12.559	37.804	38.749	1.00	156.36
	2978	CA	ARG B	174	-11.852	38.646	39.733	1.00	159.88
45	2979	CB	ARG B	174	-10.934	39.640	39.008	1.00	160.37
	2980	CG	ARG B	174	-11.660	40.518	38.000	1.00	164.23
	2981	CD	ARG B	174	-11.074	40.350	36.593	1.00	169.49
	2982 2983	NE	ARG B	174	-12.049	40.638	35.539	1.00	176.01
50	2984	CZ NH1	ARG B	174	-12.039	41.731	34.773	1.00	180.58
50	2985	NH2	ARG B ARG B	174	-11.100	42.655	34.956	1.00	179.79
-	2986	C	ARG B	174 174	-12.954 -12.853	41.882	33.824	1.00	181.42
	2987	ŏ	ARG B	174		39.368	40.639	1.00	160.54
	2988	Č1	NAG B	221	-13.891 22.996	38.80 9 15.148	41.006	1.00	159.92
55	2989	C2	NAG B	221	23.132	14.494	29.775 28.397	1.00	90.21
-	2990	N2	NAG B	221	21.968	13.691	28.083	1.00 1.00	106.23
	2991	C7	NAG B	221	21.087	14.132	27.187	1.00	110.50 109.71
	2992	07	NAG B	221	21.209	15.211	26.594	1.00	98.37
	2993	C8	NAG B	221	19.888	13.243	26.902	1.00	105.30
60	2994	C3	NAG B	221	24.395	13.644	28.376	1.00	115.44
	2995	03	NAG B	221	24.547	13.046	27.097	1.00	116.65
	2996	C4	NAG B	221	25.598	14.538	28.682	1.00	118.34
	2997	04	NAG B	221	26.785	13.757	28.731	1.00	122.24
65	2998	C5	NAG B	221	25.393	15.264	30.022	1.00	113.54
UJ	2999 3000	O5 Ce	NAG B	221	24.136	15.989	30.028	1.00	102.61
	3000	C6 O6	NAG B	221	26.494	16.278	30.269	1.00	108.41
	3002	C1	nagib Nagib	221	26.454	16.766	31.601	1.00	119.03
	3003	62	NAG B	242 242	7.596 8.393	9.421	42.304	1.00	89.99
70	3004	N2	NAG B	242	9.815	8.151 8.410	42.040	1.00	87.43
•	•	-			0.010	U.71U	42.148	1.00	86.29

	3005	C 7	NAG B	242	10.433	8.308	43.321	1.00	82.76
	3006	07	NAG B	242	9.852	7.998	44.367	1.00	76.22
	3007	C8	NAG B	242	11.928	8.599	43.333	1.00	77.25
_	3008	cs	NAG B	242	8.059	7.652	40.641	1.00	90.08
5	3009	O3	NAG B	242	8.693	6.400	40.436	1.00	97.55
	3010 3011	C4 O4	NAG B NAG B	242 242	6.539	7.501	40.426	1.00	91.14
	3011	C5	NAG B	242 242	6.283 5.757	7.380 8.728	39.009 40.956	1.00	112.32
	3013	O5	NAG B	242	6.202	9.104	42.276	1.00 1.00	82.98
10	3014	C6	NAG B	242	4.266	8,467	41.060	1.00	91.07 84.52
	3015	O6	NAG B	242	3.514	9.640	40.779	1.00	85.63
	3016	C1	NAG B	243	6.193	6.123	38.423	1.00	105.62
	3017	C2	NAG B	243	5.464	6.267	37.081	1.00	107.32
15	3018	N2	NAG B	243	4.122	6.776	37.289	1.00	101.51
13	3019 3020	C7 O7	NAG B	243	3.804	7.995	36.858	1.00	90.92
	3020	C8	NAG B NAG B	243 243	4.599 2.389	8.719 8.483	36.255	1.00	78.67
	3022	ČŠ	NAG B	243	5.435	4.929	37.120 36. 34 4	1.00 1.00	83.10
	3023	03	NAG B	243	4.817	5.094	35.073	1.00	112.30 112.99
20	3024	C4	NAG B	243	6.875	4.455	36.166	1.00	114.52
	3025	O4	NAG B	243	6.914	3.184	35.480	1.00	130.57
	3026	C5	NAG B	243	7.570	4.361	37.533	1.00	107.51
	3027	O5	NAG B	243	7.529	5.646	38.195	1.00	110.47
25	3028 3029	C6 O6	NAG B NAG B	243	9.034	3.978	37.402	1.00	100.22
23	3030	C1	MAN B	243 244	9.696 7.657	3.984 3.203	38.659	1.00	87.89
	3031	C2	MAN B	244	0.772	3.203 2.971	34. 3 07 33. 0 58	1.00 1.00	139.64
	3032	O2	MAN B	244	7.304	3.675	31.948	1.00	140.01 144.21
	3033	C3	MAN B	244	6.590	1.496	32.679	1.00	138.91
30	3034	O 3	MAN B	244	6.103	1.414	31.347	1.00	144.28
	3035	C4	MAN B	244	7.910	0.735	32.788	1.00	139.81
	3036	04	MAN B	244	7.708	-0.643	32.517	1.00	144.34
	3037	C5	MAN B	244	8.435	0.909	34.198	1.00	140.48
35	3038 3039	O5 C6	MAN B MAN B	244 244	8.779	2.294	34.406	1.00	147.09
JJ	3040	06	MAN B	244 244	9.676 10.863	0.070 0.718	34.479 34.041	1.00	136.69
	3041	C1	NAG B	335	10.865	24.720	18.959	1.00 1.00	123.90 65.94
	3042	C2	NAG B	335	12.028	24.987	17.932	1.00	79.27
40	3043	N2	NAG B	335	11.848	24.183	16.736	1.00	91.33
40	3044	C7	NAG B	335	11.340	24.727	15.629	1.00	98.55
	3045	07	NAG B	335	10.962	25.902	15.560	1.00	81.86
	3046 3047	C8 C3	NAG B	335	11.212	23.824	14.411	1.00	99.41
	3047	ος Ο3	NAG B NAG B	335 335	13.413 14.442	24.705 25.019	18.548	1.00	84.72
45	3049	Č4	NAG B	335	13.604	25.515 25.515	17.611 19.838	1.00 1.00	91.27 80.89
	3050	04	NAG B	335	14.831	25.090	20.488	1.00	64.07
	3051	C5	NAG B	335	12.419	25.265	20.794	1.00	64.08
	3052	O5	NAG B	335	11.144	25.538	20.131	1.00	71.94
50	3053	C6	NAG B	335	12.531	26.144	22.030	1.00	64.49
50	3054 3055	O6	NAG B	335	11.291	26.809	22.362	1.00	45.77
	3056	C1 C2	NAG B NAG B	336 336	15.929	25.939	20.563	1.00	97.76
	3057	N2	NAG B	336	16.577 15.705	25.748 26.270	21.946 22.982	1.00	97.78
	3058	C7	NAG B	336	15.077	25.437	23.810	1.00 1.00	97.76 97.93
55	3059	07	NAG B	336	15.179	24.203	23.741	1.00	97.68
	3060	C8	NAG B	336	14.193	26.073	24.873	1.00	97.92
	3061	C3	NAG B	336	17.943	26.425	22.064	1.00	97.90
	3062	03	NAG B	336	18.571	25.981	23.258	1.00	98.29
60	3063 3064	C4	NAG B	336	18.847	26.092	20.880	1.00	98.00
00	3065	O4 C5	NAG B NAG B	336	20.012	26.915	20. 922	1.00	97.87
	3066	O5	NAG B	336 336	18.103 16.862	26.315 25.561	19.557 19.525	1.00	97.95
	3067	C6	NAG B	336	18.956	25.835	18.400	1.00 1.00	97.83 97.91
	3068	O 6	NAG B	336	18.216	25.798	17.193	1.00	97.89
65	3069	C1	FCA B	337	11.537	27.883	23.223	1.00	97.62
	3070	C2	FCA B	337	10.367	28.129	24.189	1.00	97.53
	3071	C3	FCA B	337	9.202	28.823	23.571	1.00	97.82
	3072 3073	C4 C5	FCA B	337	9.595	30.213	22.961	1.00	97.76
70	3073 3074	C5 C6	FCA B FCA B	337 337	10.713	29.895	21.926	1.00	97.77
, ,	50/4	∨ 6	FUA B	337	11.421	31.110	21.306	1.00	97.74

	3075	02	FCA B	337	9.934	26.823	24.727	1.00	97.69
	3076	03	FCA B	337	8.162	29.022	24.541	1.00	97.99
	3077	O4	FCA B	337	10.062	31.100	24.005	1.00	97.77
_	3078	O 5	FCA B	337	11.775	29.137	22.508	1.00	97.61
5	3079	C1	NAG B	340	-0.412	38.735	24.336	1.00	122.51
	3080	C2	NAG B	340	-1.134	39.580	25.381	1.00	120.32
	3081	N2	NAG B	340	-2.513	39.812	24.998	1.00	123.12
	3082	C7	NAG B	340	-3.481	39.652	25.892	1.00	119.35
••	3083	07	NAG B	340	-3.272	39.289	27.048	1.00	117.53
10	3084	C8	NAG B	340	-4.900	39.928	25.422	1.00	119.54
	3085	СЗ	NAG B	340	-0.418	40.906	25.454	1.00	119.27
	3086	03	NAG B	340	-1.096	41.797	26.326	1.00	109.33
	3087	C4	NAG B	340	1.035	40.774	25.885	1.00	127.45
1 ~	3088	04	NAG B	340	1.546	42.148	25.882	1.00	140.24
15	3089	C5	NAG B	340	1.739	39.801	24.880	1.00	128.90
	3090	O5	NAG B	340	0.965	38.548	24.746	1.00	126.48
	3091	C6	NAG B	340	3.135	39.394	25.344	1.00	127.49
	3092	O6	NAG B	340	3.474	38.081	24.908	1.00	123.34
20	3093	Ç1	NAG B	341	2.837	42.676	25.784	1.00	149.17
20	3094	C2	NAG B	341	3.740	42.731	27.002	1.00	145.12
	3095	N2	NAG B	341	2.968	42.757	28.228	1.00	146.42
	3096	C7	NAG B	341	2.704	41.612	28.847	1.00	145.07
	3097	07	NAG B	341	3.106	40.526	28.416	1.00	132.12
25	3098	C8	NAG B	341	1.890	41.672	30.122	1.00	142.75
25	3099	C3	NAG B	341	4.552	44.017	26.806	1.00	143.92
	3100	03	NAG B	341	5.474	44.200	27.872	1.00	142.89
	3101	C4	NAG B	341	5.304	43.958	25.449	1.00	148.66
	3102	04	NAG B	341	5.954	45.201	25.210	1.00	144.18
30	3103	C5	NAG B	341	4.351	43.643	24.269	1.00	155.68
30	3104	O5	NAG B	341	3.515	42.481	24.540	1.00	161.36
	3105	C6	NAG B	341	5.092	43.354	22.983	1.00	161.88
	3106	O6	NAG B	341	4.581	44.135	21.915	1.00	165.58
	3107	C1	NAG B	366	-8.147	13.841	29.242	1.00	143.91
35	3108	C2	NAG B	366	-8.310	12.851	30.401	1.00	148.60
33	3109 3110	N2 C7	NAG B	366	-7.063	12.152	30.649	1.00	155.49
	3110	07 07	NAG B	366	-6.400	12.345	31.787	1.00	156.20
	3112	C8	NAG B	366	-6.791	13.114	32.670	1.00	152.95
	3113	C3	NAG B NAG B	366	-5.103	11.570	31.975	1.00	155.57
40	3114	O3	NAG B	366	-9.420	11.849	30.045	1.00	149.01
70	3115	03 C4	NAG B	366 366	-9. 65 8	10.967	31.133	1.00	143.79
	3116	04 04	NAG B	366	-10.713	12.593	29.696	1.00	151.07
	3117	C5	NAG B	366 366	-11.684	11.663	29.237	1.00	149.83
	3118	O5	NAG B	366	-10.447 -9.380	13.654 14.536	28.611	1.00	149.31
45	3119	C6	NAG B	366	-9.380 -11.657	14.536	29.019	1.00	146.79
73	3120	O6	NAG B	366	-11.657 -11.370		28.340	1.00	149.54
	3120	00	MAG B	300	-11.370	15.902	28.578	1.00	136.69

Table 8. Atomic coordinates of PhFceRI α_{1-172} , Form H1

	ATOM NUMBER	ATOM TYPE	RESIDUE	•	_ x _	<u>_Y_</u>	_ Z _	<u>occ</u>	_ B
	1	СВ	VAL	_					
5	2	CG1	VAL	1	53.051 52.370	36. 792 35.571	77.715	1.00	118.55
_	3	CG2	VAL	i	53.204	37.651	77.956 79.132	1.00 1.00	118.55
	4	С	VAL	1	54.467	36.682	75.485	1.00	118.55 75.78
	5	0	VAL	1	53.770	37.511	74.950	1.00	75.78
10	6	N	VAL	1	55.482	37.216	77.849	1.00	75.78
10	7 8	CA N	VAL PRO	1	54.432	36.462	77.091	1.00	75.78
	9	CD	PRO	2	55.312 56.277	35.9 5 3 34.989	74.688 75.182	1.00	130.31
	10	CA	PRO	2 2	55.477	36.015	73.162	1.00	94.32
. ~	11	СВ	PRO	2	56.190	34.719	72.910	1.00 1.00	130.31 94.32
15	12	CG	PRO	2	57.105	34.684	74.012	1.00	94.32
	13	С О	PRO	2 2 3 3	54.053	36.005	72.706	1.00	130.31
	14 15	N	PRO GLN	2	53.189	35.367	73.293	1.00	130.31
	16	CA	GLN	3	53.786 52.463	36.805 36.918	71.691 71.130	1.00	104.92
20	17	СВ	GLN	3	52.537	37.847	69.919	1.00 1.00	104.92
	18	CG	GLN	3	51.192	38.291	69.421	1.00	99.07 99.07
	19	CD	GLN	3	50.249	38.740	70.542	1.00	99.07
	20 21	OE1	GLN	3	50.548	39.683	71.287	1.00	99.07
25	22	NE2 C	GLN GLN	3	49.101	38.061	70.664	1.00	99.07
	23	ŏ	GLN	3 3	52.005 52.779	35.499 34.545	70.762	1.00	104.92
	24	Ň	LYS	4	50.747	35.334	70.877 70.360	1.00 1.00	104.92
	25	CA	LYS	4	50.255	33.998	69.981	1.00	70.29 70.29
20	26	СВ	LYS	4	48.731	33.942	70.002	1.00	91.56
30	27	CG	LYS	4	47.997	34.836	69.020	1.00	91.56
	28 29	CD CE	LYS LYS	4	46.591	34.284	68.830	1.00	91.56
	30	NZ	LYS	4	45.661 45.296	35.309 36.401	68.214	1.00	91.56
	31	Ċ	LYS	4	50.735	33.524	69.165 68.613	1.00 1.00	91.56
35	32	0	LYS	4	50.793	34.314	67.654	1.00	70.29 70.29
	33	N	PRO	5 5	51. 05 6	32.216	68.503	1.00	78.97
	34	CD	PRO	5	51.154	31.280	69.6 3 3	1.00	108.62
	35 36	CA CB	PRO PRO	5	51.541	31.566	67.284	1.00	78.97
40	37	CG	PRO	5 5	51.808 52.211	30.127 30.315	67.739	1.00 1.00	108.62
	38	Č	PRO	5	50.601	31.638	69.151 66.091	1.00 1.00	108.62 78.97
	39	0	PRO	5	49.439	32.036	66.221	1.00	78.97 78.97
	40	N	LYS	6	51.124	31.294	64.916	1.00	88.04
45	41 42	CA	LYS	6	50.283	31.336	63.731	1.00	88.04
73	43	CB CG	LYS LYS	6	50.440	32.681	63.010	1.00	139.11
	44	CD	LYS	6 6	49.189 49.300	33.108 34.555	62.233	1.00	i39.11
	45	CE	LYS	6	47.998	35.105	61.830 61.293	1.00 1.00	139.11
~~	46	NZ	LYS	6	48.130	36.569	61.033	1.00	139.11 139.11
50	47	C	LYS	6	50.598	30.191	62.780	1.00	38.04
	48 49	0	LYS	6	51.765	29.850	62.565	1.00	88.04
	50	N CA	VAL VAL	7	49.539	29.590	62.235	1.00	50.50
	51	CB	VAL	7	49.660 48.471	28.476 27.522	61.307	1.00	50.50
55	52	CG1	VAL	7	48.757	26.276	61.411 60.577	1.00 1.00	69.58 69.58
	53	CG2	VAL	7	48.212	27.169	62.858	1.00	69.58
	54	C	VAL	7	49.733	28.947	59.871	1.00	50.50
	55 56	0	VAL	7	48.997	29.831	59.446	1.00	50.50
60	50 57	N CA	SER SER	8	50.597	28.301	59.112	1.00	106.26
-	58	CB	SER	8 8	50.788 52.121	28.646 29.344	57.723 57.569	1.00	106.26
	59	OG.	SER	8	53.155	28.427	57.568 57.902	1.00 1.00	69.57 69.57
	60	С	SER	8	50.816	27.357	56. 93 3	1.00	106.26
45	61	0	SER	8	51.370	26.353	57.380	1.00	106.26
65	62 63	N	LEU	9	50.221	27.381	55.754	1.00	69.51
	64	CA CB	LEU LEU	9 9	50.212	26.187	54.937	1.00	69.51
		00	LEU	.	48.809	25.862	54.432	1.00	46.80

	65 66	CG CD1	LEU	9 .	47.549	26.374	55.111	1.00	46.80
	67	CD2	LEU	. 9	46.349 47.523	25.850 25.926	54.373	1.00	46.80
	68	Č	LEU	9	51.111	26.317	56.559 53.718	1.00 1.00	46.80
5	69	Ŏ	LEU	9	51.229	27.385	53.110	1.00	69.51
	70	N	ASN	10	51.725	25.199	53.358	1.00	69.51 65.02
	71	ÇA	ASN	10	52.576	25.120	52.197	1.00	65.02
	72	СВ	ASN	10	54.050	25.035	52.622	1.00	82.93
10	73	CG	ASN	10	54.979	24.700	51.475	1.00	82.93
10	74 75	OD1 ND2	ASN ASN	10	54.991	25.378	50.451	1.00	82.93
	76	C	ASN	10 10	55.771 52.130	23.650	51.643	1.00	82.93
	77	ŏ	ASN	10	52.130	23.839 22.728	51.492 51.953	1.00	65.02
	78	Ň	PRO	11	51.306	23.967	50.430	1.00 1.00	65.02
15	79	CD	PRO	11	50.772	22.738	49.827	1.00	60.91 59.89
	60	CA	PRO	11	50.786	25.157	49.733	1.00	60.91
	81	CB	PRO	11	49.977	24.568	48.583	1.00	59.89
	82	CG	PRO	11	50.471	23.159	48.449	1.00	59.89
20	83 84	c o	PRO PRO	11 11	49.881	26.032	50.613	1.00	60.91
20	85	Ň	PRO	12	49.435 49.570	25 ^ '8	51.675	1.00	60.91
	86	ČD	PRO	12	50.133	27.245 27.764	50.142 48.895	1.00 1.00	78.15
	87	CA	PRO	12	48.728	28.264	50.791	1.00	41.22 78.15
0.5	88	СВ	PRO	12	48.984	29.528	49.967	1.00	41.22
25	89	ÇG	PRO	12	50.225	29.226	49.207	1.00	41.22
	90	C	PRO	12	47.264	27.890	50.704	1.00	78.15
	91 92	0 N	PRO	12	46.420	28.401	51.437	1.00	78.15
	93	OA	TRP TRP	13 13	46.975	27.001	49.773	1.00	63.58
30	94	CB	TRP	13	45.621 45.619	26.563 25.679	49.541	1.00	63.58
	95	CG	TRP	13	46.483	26.211	48.308 47.211	1.00	43.81
	96	CD2	TRP	13	46.444	27.519	46.634	1.00 1.00	43.81 43.81
	97	CE2	TRP	13	47.339	27.524	45.549	1.00	43.81
25	98	CE3	TRP	13	45.732	28.687	46.926	1.00	43.81
35	99	CD1	TRP	13	47.385	25.507	46.480	1.00	43.81
	100 101	NE1	TRP	13	47.903	26.281	45.477	1.00	43.81
	102	CZ2 CZ3	TRP TRP	13 13	47.543	28.650	44.746	1.00	43.81
	103	CH2	TRP	13	45.935 46.838	29.812 29.780	46.128	1.00	43.81
40	104	Ċ	TRP	13	45.032	25.822	45.046 50.730	1.00 1.00	43.81 63.58
	105	0	TRP	13	45.556	24.777	51.137	1.00	63.58
	106	N.	ASN	14	43.947	26.377	51.280	1.00	73.67
	107	CA	ASN	14	43.239	25.781	52.412	1.00	73.67
45	108 109	CB	ASN	14	42.720	26.868	53.362	1.00	86.63
73	110	CG OD1	ASN ASN	14	41.638	27.726	52.745	1.00	86.63
	111	ND2	ASN	14 14	41.780 40.548	28.226 27.912	51.630	1.00	86.63
	112	C	ASN	14	42.090	24.940	53.477 51.861	1.00 1.00	86.63
	113	0	ASN	14	41.276	24.409	52.609	1.00	73.67 73.67
50	114	N	ARG	15	42.045	24.837	50.534	1.00	50.70
	115	CA	ARG	15	41.058	24.054	49.800	1.00	50.70
	116	CB	ARG	15	40.174	24.947	48.943	1.00	57.52
	117 118	CG CD	ARG	15	39.558	26.093	49.674	1.00	57.52
55	119	NE	ARG ARG	15 15	38.636	26.850	48.745	1.00	57.52
	120	cz	ARG	15	37.242 36.364	26.435 26.620	48.833	1.00	57.52
	121	NH1	And	15	36.752	27.189	47.853 46.730	1.00 1.00	57.52 57.52
	122	NH2	ARG	15	35.093	26.286	47.999	1.00	57.52 57.52
<i>c</i> 0	123	С	ARG	15	41.851	23.139	48.858	1.00	50.70
60	124	0	ARG	15	42.427	23.596	47.863	1.00	50.70
	125	N.	ILE	16	41.902	21.849	49.150	1.00	58.15
	126 127	CA CB	ILE	16	42.633	20.980	48.254	1.00	58.15
	128	CB CG2	ILE	16	43.956	20.548	48.866	1.00	51.72
65	129	CG1	ILE	16 16	44.934 43.718	21.703	48.821	1.00	51.72
	130	CD1	ILE	16	43.718 44.968	20.052 19.557	50.287	1.00	51.72
	131	Č.	ILE	16	41.839	19.761	50.978 47.876	1.00 1.00	51.72 58.15
	132	0	ILE	16	40.875	19.403	47.670 48.540	1.00	58.15 58.15
70	133	N	PHE	17	42.260	19.157	46.776	1.00	58.19
70	134	CA	PHE	17	41.660	17.957	46.241	1.00	58.19
				•					

	135 136	CB CG	PHE	17 ·	42.213	17.669	44.860	1.00	25.51
	136	CD1:	PHE PHE	17	41.536	18.414	43.776	1.00	25.51
	138	CD2	PHE	17 17	42.250 40.171	18.820	42.639	1.00	25.51
5	139	CE1	PHE	17	41.608	18.682 19.487	43.857	1.00	25.51
_	140	CE2	PHE	17	39.532	19.344	41.592 42.825	1.00 1.00	25.51
	141	CZ	PHE	17	40.253	19.752	41.673	1.00	25.51 25.51
	142	С	PHE	17	42.019	16.789	47,117	1.00	23.51 58.19
••	143	0	PHE	17	43.030	16.815	47.836	1.00	58.19
10	144	N	LYS	18	41.202	15.749	47.024	1.00	64.21
	145	CA	LYS	18	41.421	14.528	47.770	1.00	64.21
	146 147	CB CG	LYS	18	40.266	13.572	47.476	1.00	120.30
	148	CD	LYS LYS	18	40.180	12.351	48.352	1.00	120.30
15	149	CE	LYS	18 18	38.856 38.656	11.639 10.437	48.078	1.00	120.30
	150	NZ	LYS	18	39.547	9.324	48.983 48.594	1.00	120.30
	151	C	LYS	18	42.740	13.978	47.237	1.00 1.00	120.30 64.21
	152	0	LYS	18	42.970	13.995	46.027	1.00	64.21
20	153	N	GLY	19	43.619	13.536	48.134	1.00	59.20
20	154	CA	GLY	19	44.893	12.963	47.706	1.00	59.20
	155	C	GLY	19	46.112	13.851	47.506	1.00	59.20
	156 157	0 N	GLY GLU	19 20	47.199	13.352	47.174	1.00	59.20
	158	CA	GLU	20	45.938 47.046	15.156 16.087	47.686	1.00	96.38
25	159	СВ	GLU	20	46.547	17.429	47.539 46.993	1.00	96.38
	160	ÇĠ	GLU	20	45.820	17.303	45.661	1.00 1.00	62.66
	161	CD	GLU	20	45.468	18.648	45.025	1.00	62.66 62.66
	162	OE1	GLU	20	44.899	19.525	45.726	1.00	62.66
30	163	OE2	GLU	20	45.754	18.811	43.815	1.00	62.66
JU	164 165	C	GLU	20	47.666	16.261	48.917	1.00	96.38
	166	0 N	GLU ASN	20	47.055	15.899	49.922	1.00	96.38
	167	CA	ASN	21 21	48.886 49.550	16.783 16.992	48.966	1.00	82.14
	168	CB	ASN	21	50.929	16.375	50.245 50.212	1.00 1.00	82.14
35	169	CG	ASN	21	50.907	15.025	49.599	1.00	83.98 83.98
	170	OD1	ASN	21	50.088	14.203	49.969	1.00	83.98
	171	ND2	ASN	21	51.791	14.775	48.651	1.00	83.98
	172	C	ASN	21	49.661	18.458	50.598	1.00	82.14
40	173 174	0 N	ASN VAL	21	49.706	19.317	49.727	1.00	82.14
10	175	CA	VAL	22 22	49.715 49.809	18.739 20.109	51.889	1.00	82.30
	176	CB	VAL	22	48.407	20.695	52.347 52.489	1.00	82.30
	177	CG1	VAL.	22	47.687	19.993	53.637	1.00 1.00	52.62 52.62
4 5-	178	CG2	VAL	22	48.473	22.229	52.679	1.00	52.62
45	179	Ç	VAL	22	50.502	20.090	53.698	1.00	82.30
	180	0	VAL	22	50.248	19.192	54.503	1.00	82.30
	181 182	N CA	THR THR	23	51.376	21.063	53. 95 4	1.00	73.57
	183	ČB	THR	23 23	52.083 53.598	21.109	55.231	1.00	73.57
50	184	OG1	THA .	23	54.021	21.205 20.223	55.035 54.076	1.00 1.00	78.82
	185	CG2	THR	23	54.309	20.974	56.380	1.00	78.82 78.82
	186	С	THR	23	51.658	22.281	56.097	1.00	76.62 73.57
	187	0	THR	23	51.549	23.407	55.618	1.00	73.57
55	188	N	LEU	24	51.417	22.007	57.374	1.00	80.82
JJ	189 190	CA	LEU	24	51.026	23.040	58.314	1.00	80.82
	191	CB CG	LEU LEU	24	49.818	22.605	59.138	1.00	72.07
	192	CD1	LEU	24 24	48.578 47.353	22.217 22.285	58.346	1.00	7 <u>2</u> .07
	193	CD2	LEU	24	48.412	23.157	59.242 57.182	1.00	72.07
60	194	C	LEU	24	52.188	23.322	59.239	1.00 1.00	72.07 80.82
	195	0	LEU	24	52.771	22.420	59.825	1.00	80.82
	196	N	THR	25	52.527	24.591	59.367	1.00	57.44
	197	CA	THR	25	53.622	24.995	60.228	1.00	57.44
65	198 199	CB	THR	25	54.748	25.593	59.431	1.00	58.08
<i>55</i>	200	OG1 CG2	THR	25 25	55.299	24.593	58.568	1.00	58.08
	201	C	THR THR	25 25	55.812 53.197	26.103	60.372	1.00	58.08
	202	ŏ	THR	25 25	52.524	26.039 27.007	61.238	1.00	57.44
	203	N	CYS	26	53.589	25.833	60.891 62.489	1.00 1.00	57.44 94.33
70	204	CA	CYS	26	53.276	26.780	63.551	1.00	94.33
									J 1.00

	205 206	C	CYS	26 ⁻	54.464	27.725	63.557	1.00	94.33
	206	O CB	CYS	26 26	55.604 53.206	27.267	63.459	1.00	94.33
	208	SG	CYS	26 26	53.206 52.191	26.060 26.860	64.890 66.176	1.00	89.97
5	209	Ň	ASN	27	54.229	29.031	63.651	1.00 1.00	89.97
_	210	CA	ASN	2 7	55.363	29.941	63.665	1.00	88.38 88.38
	211	СВ	ASN	27	55.584	30.555	62.273	1.00	163.21
	212	CG	ASN	27	56.225	29.574	61.290	1.00	163.21
10	213	OD1	ASN	27	57.082	28.768	61.667	1.00	163.21
10	214	ND2	ASN	27	55.825	29.654	60.020	1.00	163.21
	215 216	CO	ASN	27	55.336	31.039	64.719	1.00	88.38
	217	N	ASN GLY	27 28	54.563 56.164	31.989 30.862	64.641	1.00	88.38
	218	CA	GLY	28	56.306	31.863	65.736 66.769	1.00 1.00	157.55
15	219	C	GLY	28	57.695	32.269	66.353	1.00	157.55 157.55
	220	0	GLY	28	58.644	31.591	66.702	1.00	157.55
	221	N	ASN	29	57.813	33.337	65.572	1.00	155.07
	222	CA	ASN	29	59.110	33.779	65.057	1.00	155.07
20	223	CB	ASN	29	59.054	35.252	64.655	1.00	162.85
20	224 225	CG OD1	ASN ASN	29 29	57.897 57.726	35.564	63.723	1.00	162.85
	226	ND2	ASN	29	57.735 57.088	34.939 36.545	62.672 64.103	1.00	162.85
	227	C	ASN	29	60.312	33.547	65.963	1.00 1.00	162.85
	228	Ŏ	ASN	29	61.386	33.183	65.471	1.00	155.07 155.07
25	229	N	ASN	30	60.152	33.787	67.269	1.00	156.06
	230	CA	ASN	30	61.241	33.545	68.220	1.00	156.06
	231	CB	ASN	30	60.696	33.490	69.653	1.00	177.59
	232	CG	ASN	30	60.720	34.850	70.334	1.00	177.59
30	233 234	OD1 ND2	ASN ASN	30	61.733	35.550	70.290	1.00	177.59
30	235	C	ASN	30 30	59.613 61.697	35.227 32.182	70.970	1.00	177.59
	236	ŏ	ASN	30	62.886	31.932	. 67.729 67.477	1.00 1.00	156.06
	237	Ň	PHE	31	60.702	31.316	67.577	1.00	156.06 152.23
	238	CA	PHE	31	60.896	30.010	66.990	1.00	152.23
35	239	CB	PHE	31	61.081	30.267	65.497	1.00	158.06
	240	CG	PHE	31	60.650	29.154	64.612	1.00	158.06
	241	CD1	PHE	31	59.315	28.746	64.550	1.00	158.06
	242 243	CD2 CE1	PHE	31	61.573	28.561	63.769	1.00	158.06
40	243 244	CE2	PHE PHE	31 31	58.924 61.197	27.755 27.579	63.653	1.00	158.06
	245	CZ	PHE	31	59.869	27.173	62.877 62.810	1.00 1.00	158.06 158.06
	246	Č	PHE	31	62.099	29.281	67.576	1.00	152.23
	247	0	PHE	31	62.836	28.610	66.857	1.00	152.23
4-	248	N	PHE	32	62.304	29.414	68.880	1.00	166.63
45	249	CA	PHE	32	63.432	28.752	69.510	1.00	166.63
	250	CB	PHE	32	63.802	29.479	70.792	1.00	178.95
	251 252	CG CD1	PHE	32	64.123	30.923	70.567	1.00	178.95
	253	CD2	PHE PHE	32 32	63.361 65.174	31.922 31.288	71.164	1.00	178.95
50	254	CE1	PHE	32	63.631	33.271	69.723 70.914	1.00 1.00	178.95
	255	CE2	PHE	32	65.452	32.634	69.466	1.00	178.95 178.95
	256	CZ	PHE	32	64.681	33.629	70.068	1.00	178.95
	257	С	PHE	32	63.116	27.288	69.760	1.00	166.63
55	258	0	PHE	32	63.884	26.5 6 7	70.399	1.00	166.63
55	259	N	GLU	33	61.968	26.864	69.239	1.00	156.85
	260 261	CA CB	GLU GLU	33 33	61.527	25.475	69.315	1.00	156.85
	262	CG	GLU	33	62.558 63.153	24.582 25.157	68.620 67.220	1.00	168.05
	263	CD	GLU	33	64.130	24.188	67.330 66.704	1.00 1.00	168.05
60	264	OE1	GLU	33	64.854	23.526	67.477	1.00	168.05 168.05
	265	OE2	GLU	33	64.175	24.084	65.461	1.00	168.05
	266	Ç	GLU	33	61.233	24.913	70.708	1.00	156.85
	267	0	GLU	33	60.369	24.046	70.851	1.00	156.85
65	268	N	VAL	34	61.963	25.376	71.719	1.00	106.92
O)	269 270	CA CB	VAL	34	61.748	24.926	73.095	1.00	106.92
	270 271	CB CG1	VAL VAL	34 34	60.953	25.998 25.626	73.882	1.00	129.93
	272	CG2	VAL	34 34	60.864 61.607	25.626 27.359	75.361 73.695	1.00	129.93
	273	c	VAL.	34	61.011	23.573	73.095 73.211	1.00 1.00	129.93 106.92
70	274	Ō	VAL	34	59.825	23.521	73.562	1.00	106.92
				•					.00.02

	275	N	SER	35	61.712	22.490	72.883	4.00	470.50
	276	CA	SER	35	61.170	21.135	72.978	1.00 1.00	178.50 178.50
	277	CB:	SER	35	60.683	20.879	74.409	1.00	177.04
	278	OG '	SER	35	61.781	20.767	75.302	1.00	177.04
5	279	Ç	SER	35	60.102	20.645	71.988	1.00	178.50
	280	0	SER	35	60.449	20.069	70.956	1.00	178.50
	281 282	N GA	SER SER	36 36	58.816	20.858	72.286	1.00	97.16
	283	CB	SER	36	57.742 57.175	20.347 19.038	71.411 71.993	1.00 1.00	97.16
10	284	OG	SER	36	58.160	18.018	72.059	1.00	145.01
	285	Ċ	SER	36	56.560	21.259	71.061	1.00	145.01 97.16
	286	0	SER	36	56.405	22.357	71.604	1.00	97.16
	287	N	THR	37	55.725	20.750	70.149	1.00	111.12
15	288	CA	THR	37	54.530	21.433	69.638	1.00	111.12
15	289 290	CB OG1	THR THR	37 37	54.686	21.780	68.144 67.054	1.00	142.34
	291	CG2	THR	37 37	55.863 53.465	22.572 22.536	67.954 67. 638	1.00 1.00	142.34
	292	Č	THR	37	53.273	20.565	69.746	1.00	142.34 111.12
••	293	0	THR	37	53.323	19.357	69.509	1.00	111.12
20	294	N	LYS	38	52.147	21.193	70.075	1.00	89.74
	295	CA	LYS	38	50.879	20.480	70.195	1.00	89.74
	296 297	CB CG	LYS LYS	38	50.253	20.739	71.559	1.00	101.72
	298	CD	LYS	38 38	50.833 50.223	19.880 20,211	72.648 73.991	1.00	101.72
25	299	CE	LYS	38	50.893	19.410	75.110	1.00 1.00	101.72 101.72
	300	NZ	LYS	38	50.571	19.965	76.465	1.00	101.72
	301	Ç	LYS	38	49.889	20.878	69.112	1.00	89.74
	302	0	LYS	38	49.478	22.036	69.039	1.00	89.74
30	303 304	N CA	TRP	39	49.501	19.911	68.280	1.00	92.70
50	305	CA CB	TRP TRP	39 39	48.549 48.948	20.162 19.417	67.196	1.00	92.70
	306	ČG	TRP	39	50.148	19.958	65.933 65.279	1.00 1.00	89.95 89.95
	307	CD2	TRP	39	50.188	21.016	64.329	1.00	89.95
0.5	308	CE2	TRP	39	51.536	21.192	63.941	1.00	89.95
35	309	CE3	TRP	39	49.211	21.846	63.759	1.00	89.95
	310 311	CD1	TRP	39	51.438	19.535	65.441	1.00	89.95
	312	NE1 CZ2	TRP TRP	39 39	52.282 51.938	20.269 22.145	64.639	1.00	89.95
	313	CZ3	TRP	39	49.603	22.145 22.799	63.017 62.839	1.00 1.00	89.95 89.95
40	314	CH2	TRP	39	50.958	22.943	62.475	1.00	89.95
	315	C	TRP	39	47.139	19.743	67.541	1.00	92.70
	316	0	TRP	39	46.926	18.717	68.177	1.00	92.70
	317 318	N	PHE	40	46.167	20.522	67.096	1.00	74.21
45	319	CA CB	PHE PHE	40 40	44.782 44.177	20.188 21.186	67.382	1.00	74.21
10	320	CG	PHE	40	44.868	21.100 21.229	68.365 69.698	1.00 1.00	91.61 91.61
	321	CD1	PHE	40	46.143	21.793	69.829	1.00	91.61
	322	CD2	PHE	40	44.231	20.730	70.833	1.00	91.61
50	323	CE1	PHE	40	46.761	21.876	71.069	1.00	91.61
JU	324 325	CE2 CZ	PHE	;0	44.839	20.807	72.078	1.00	91.61
	325 326	c c	PHE PHE	40 40	46.110 43.946	21.379	72.196	1.00	91.61
	327	ŏ	PHE	40	43.709	20.149 21.176	66.121 65.474	1.00	74.21
	328	Ñ	HIS	41	43.506	18.948	65.774	1.00 1.00	74.21 72.61
55	329	CA	HIS	41	42.691	18.750	64.593	1.00	72.61
	330	CB	HIS	41	43.15C	1 7.481	63.880	1.00	96.01
	331	CG	HIS	41	42.346	17.151	62.661	1.00	96.01
	332 333	CD2 ND1	HIS HIS	41	42.300	16.023	61.911	1.00	96.01
60	334	CE1	HIS	41	41.489 40.942	18.048 17.489	62.073 61.005	1.00 1.00	96.01
	335	NE2	HIS	41	41.419	16.264	60.887	1.00	96.01 96.01
	336	C	HIS	41	41.223	18.646	64.999	1.00	72.61
	337	0	HIS	41	40.831	17.703	65.698	1.00	72.61
65	338	N	ASN	42	40.419	19.616	64.563	1.00	65.96
UJ	339 340	CA C8	ASN	42 42	38.998	19.638	64.896	1.00	65.96
	341	œ	ASN ASN	42 42	38.304 37.832	18.373 18.533	64.347 63.807	1.00	107.42
	342	OD1	ASN	42	38.115	19.550	62.897 62.262	1.00 1.00	107.42 107.42
=-	343	ND2	ASN	42	37.110	17.532	62.380	1.00	107.42
70	344	С	ASN	42	38.869	19.713	66.422	1.00	65.96
				•				-	

	345	0	ASN	42 -	37.863	19.297	67.008	1.00	65.96
	346 347	N CA:	GLY GLY	43 43	39.916	20.229	67.058	1.00	142.69
	348	C.	GLY	43 43	39.930 40.418	20.362 19.152	68.505 69.292	1.00	142.69
5	349	ŏ	GLY	43	40.304	19.125	70.508	1.00 1.00	142.69
	350	Ň	SER	44	40.972	18.149	68.621	1.00	142.69 82.57
	351	CA	SER	44	41.448	16.960	69.318	1.00	82.57
	352	СВ	SER	44	40.876	15.716	68.658	1.00	65.56
10	353	og .	SER	44	41.042	14.585	69.496	1.00	65.56
10	354	C	SER	44	42.966	16.877	69.294	1.00	82.57
	355 356	O N	SER LEU	44	43.558	16.765	68.218	1.00	82.57
	357	CA	LEU	45 45	43.601 45.056	16.910 16.846	70.464	1.00	83.34
	358	CB	LEU	45	45.586	16.632	70.490 71.930	1.00 1.00	83.34
15	359	ĊĠ	LEU	45	47.121	16.657	71.530	1.00	79.17 79.17
	360	CD1	LEU	45	47.758	17.921	71.590	1.00	79.17 79.17
	361	CD2	LEU	45	47.403	16.581	73.681	1.00	79.17
	362	C	LEU	45	45.537	15.736	69.542	1.00	83.34
20	363	0	LEU	45	45.074	14.588	69.585	1.00	83.34
20	364 365	N CA	SER	46	46.447	16.125	68.658	1.00	133.67
	366	CA CB	SER SER	46 46	47.037	15.236	67.671	1.00	133.67
	367	OG	SER	46 46	47.551 48.435	16.059 15.315	66.487	1.00	75.61
	368	č	SER	46	48.196	14.486	65.662 68.299	1.00 1.00	75.61
25	369	ō	SER	46	48.864	15.000	69.195	1.00	133.67 133.67
	370	N	GLU	47	48.431	13.268	67.827	1.00	113.73
	371	CA	GLU	47	49.545	12.470	68.329	1.00	113.73
	372	CB	GLU	47	49.354	10.985	67.982	1.00	165.00
30	373	CG	GLU	47	48.217	10.318	68.775	1.00	165.00
30	374	CD	GLU	47	48.093	8.817	68.530	1.00	165.00
	375 376	OE1 OE2	GLU GLU	47 47	47.813	8.412	67.380	1.00	165.00
	377	C	GLU	47	48.270 50.821	8.039 13.023	69.494	1.00	165.00
	378	ŏ	GLU	47	51.921	12.506	67.695 67.908	1.00 1.00	113.73
35	379	Ň	GLU	48	50.650	14.089	66.915	1.00	113.73 132.93
	380	CA	GLU	48	51.755	14.763	66.249	1.00	132.93
	381	СВ	GLU	48	51.264	15.424	64.966	1.00	192.46
	382	CG	GLU	48	52.348	16.113	64.173	1.00	192.46
40	383 384	CD	GLU	48	52.450	15.579	62.762	1.00	192.46
+0	385	OE1 OE2	GLU GLU	48	51.665	14.672	62.406	1.00	192.46
	386	C	GLU	48 48	53.316 52.280	16.062 15.826	62.005	1.00	192.46
	387	ŏ	GLU	48	51.506	16.635	67.207 67.730	1.00 1.00	132.93
	388	Ñ	THR	49	53.591	15.827	67.436	1.00	132.93 120.56
45	389	CA	THR	49	54.193	16.789	68.350	1.00	120.56
	390	СВ	THR	49	54.823	16.075	69.569	1.00	154.93
	391	OG1	THR	49	55.638	14.984	69.123	1.00	154.93
	392 393	CG2	THR	49	53.740	15.552	70.504	1.00	154.93
50	394	CO	THR THR	49 40	55.248	17.684	67.713	1.00	120.56
50	395	Ň	ASN	49 50	55. 697 55. 63 9	18.652 17.368	68.323	1.00	120.56
	396	ČA	ASN	50	56.646	18.154	66.484 65.779	1.00 1.00	120.79
	397	СВ	ASN	50	57.190	17.349	64.596	1.00	120.79 183.19
	398	CG	ASN	50	57.793	16.024	65.035	1.00	183.19
55	399	OD1	ASN	50	58.218	15.900	66.182	1.00	183.19
	400	ND2	ASN	50	57.865	15.054	64.124	1.00	183.19
	401 402	C	ASN	50	56.070	19.485	65.312	1.00	120.79
	403	0 N	ASN SER	50 51	54.854	19.616	65.160	1.00	120.79
60	404	CA	SER	51	56.944 56.522	20.466 21.811	65.084 64.657	1.00	104.18
	405	CB	SER	51	57.735	22.751	64.577	1.00 1.00	104.18 100.13
	406	OG	SER	51	58.559	22.431	63.468	1.00	100.13
	407	С	SER	51	55.753	21.880	63.329	1.00	104.18
C F	408	0	SER	51	55.086	22.879	63.053	1.00	104.18
65	409	N	SER	52	55.858	20.835	62.507	1.00	108.20
	410 411	CA	SER	52 53	55.154	20.803	61.223	1.00	108.20
	412	CB OG	SER SER	52 52	56.131	20.860	60.041	1.00	83.34
	413	C	SER	52 52	56.705 54.291	22.151 19.566	59.913	1.00	83.34
70	414	ŏ	SER	52 52	54.750	18.445	61.083 61.284	1.00	108.20
					00		01.204	1.00	108.20

	415 416	N CA	LEU	53 53	53.038 52.057	19. 79 0 18. 73 0	60.720 60.536	1.00 1.00	62.72 62.72
	417	CB.	LEU	53	50.730	19.214	61.130	1.00	43.93
5	418 419	CG CD1	LEU	53	49.456	18.379	61.050	1.00	43.93
3	420	CD2	LEU	53 53	49.665 48.305	17.079	61.786	1.00	43.93
	421	C	LEU	53 53	51.912	19.148 18.398	61.680	1.00	43.93
	422	ŏ	LEU	53	51.470	19.226	59.035 58.234	1.00 1.00	62.72
	423	N	ASN	54	52.294	17.192	58.642	1.00	62.72 92.98
10	424	CA	ASN	54	52.183	16.832	57.236	1.00	92.98
	425	CB	ASN	54	53.404	16.036	56. 796	1.00	86.69
	426	CG	ASN	54	54.670	16.844	56.872	1.00	86.69
	427 428	OD1 ND2	ASN	54	54.805	17.866	56.186	1.00	86.69
15	429	C ND2	ASN ASN	54 54	55.608	16.406	57.717	1.00	86.69
	430	ŏ	ASN	54	50.941 50.701	16.029 14.991	56 .929 57 .529	1.00	92.98
	431	Ň	ILE	5 5	50.144	16.523	55.995	1.00 1.00	92.98 45.24
	432	CA	ILE	55	48.935	15.823	55.582	1.00	45.24 45.24
20	433	СВ	ILE	55	47.716	16.773	55.491	1.00	31.24
20	434	CG2	ILE	55	46.623	5.157	54.647	1.00	31.24
	435	CG1	ILE	55	47.183	17.072	56. 884	1.00	31.24
	436 437	CD1	ILE	5 5	45.969	17.961	56.867	1.00	31.24
	438	C O	ILE	55 55	49.224 49.262	15.251 15.977	54.200	1.00	45.24
25	439	Ň	VAL	56	49.437	13.942	53.201	1.00	45.24
	440	CA	VAL	56	49.730	13.244	54.1 6 0 52. 923	1.00 1.00	82.87
	441	CB	VAL	56	50.831	12.192	53.155	1.00	82.87 72.67
	442	CG1	VAL	56	51.176	11.489	51.856	1.00	72.67
20	443	CG2	VAL	56	52.057	12.862	53.731	1.00	72.67
30	444	C	VAL	56	48.467	12.569	52.398	1.00	82.87
	445 446	O N	VAL	56	47.689	12.010	53.171	1.00	82.87
	447	CA	ASN ASN	57 57	48.268	12.636	51.085	1.00	59.63
	448	CB	ASN	57 57	47.099 47.302	12.059 10.562	50.438	1.00	59.63
35	449	ČĠ	ASN	57	48.632	10.237	50.308 49. 65 5	1.00 1.00	98.65
	450	OD1	ASN	57	48.980	10.808	48.609	1.00	98.65 98.65
	451	ND2	ASN	57	49.391	9.331	50.267	1.00	98.65
	452	Ç	ASN	57	45.864	12.412	51.249	1.00	59.63
40	453 454	0	ASN	57	45.322	11.593	51.998	1.00	59.63
40	454 455	N CA	ALA	58	45.443	13.665	51.090	1.00	71.80
	456	CB	ALA ALA	58 58	44.300 43.991	14.216	51.809	1.00	71.80
	457	C	ALA	58	43.073	15.617 13.358	51.310 51.690	1.00	87.99
	458	Ö	ALA	58	42.783	12.818	50.625	1.00 1.00	71.80 71.80
45	459	N	LYS	59	42.363	13.240	52.805	1.00	71.80
	460	CA	LYS	59	41.128	12.467	52.885	1.00	72.92
	461	CB	LYS	59	41.293	11.281	53.830	1.00	124.59
	462 463	CG	LYS	59	42.422	10.361	53.457	1.00	124.59
50	463 464	CD CE	LYS LYS	59 50	42.480	9.187	54.387	1.00	124.59
50	465	NZ.	LYS	59 59	43.356 43.282	8.128	53.783	1.00	124.59
	466	Č	LYS	59	40.082	6.869 13.397	54. 5 61 53.457	1.00	124.59
	467	Ö	LYS	59	40.356	14.132	54.401	1.00 1.00	72.92 72.93
	468	N	PHE	60	38.887	13.381	52.897	1.00	72.92 56.87
55	469	CA	PHE	60	37.848	14.255	53.416	1.00	56.87
	470	СВ	PHE	60	36.488	13.707	53.028	1.00	109.01
	471	CG	PHE	60	36.29?	13.613	51. 562	1.00	109.01
	472 473	CD1 CD2	PHE	60	35.499	12.629	51.015	1.00	109.01
60	474	CE1	PHE	60 60	36.957 35.336	14.485 12.536	50.714	1.00	109.01
	475	CE2	PHE	60	36.803	14.404	49.634 49.337	1.00 1.00	109.01
	476	CZ	PHE	60	36.006	13.414	48.793	1.00	109.01 109.01
	477	С	PHE	60	37.930	14.414	54.928	1.00	56.87
C E	478	0	PHE	60	37.628	15.478	55.475	1.00	56.87
65	479	N	GLU	61	38.352	13.350	55.598	1.00	64.50
	480	CA	GLU	61	38.460	13.336	57.054	1.00	64.50
	481 482	CB CG	GLU	61	38.892	11.953	57.542	1.00	154.96
	483	CD	GLU	61 61	37.855 37.517	10.870	57.334 55.034	1.00	154.96
70	484	OE1	GLU	61	37.517 38.443	10.655 10.355	55.871 55.087	1.00	154.96
				•		10.000	55.567	1.00	154.96

	485 486 487	OE2 C O	GLU GLU	61 ⁻ 61 61	36.328 39.436 39.351	10.784 14.356 14.765	55.505 57.576	1.00	154.96 64.50
	488	Ň	ASP	62	40.371	14.745	58.731 56.713	1.00	64.50
5	489	CA	ASP	62	41.404	15.723	57.035	1.00 1.00	71.49
	490	СВ	ASP	62	42.574	15.543	56.079	1.00	71.49 78.68
	491	CG	ASP	62	43.412	14.316	56.422	1.00	78.68
	492	OD1	ASP	62	43.641	14.093	57.639	1.00	78.68
10	493	OD2	ASP	62	43.851	13,594	55.485	1.00	78.68
10	494 495	C	ASP ASP	62	40.883	17.160	57.000	1.00	71.49
	496	Ň	SER	62 63	41.574 39.654	18.102 17.326	57.400	1.00	71.49
	497	ĊA	SER	63	39.056	18.637	56.523 56.490	1.00 1.00	52.56
	498	СВ	SER	63	37.722	18.586	55.773	1.00	52.56 54.10
15	499	OG	SER	63	37.914	18.110	54.456	1.00	54.10
	500	Ç	SER	63	38.850	19.020	57. 9 36	1.00	52.56
	501	0	SER	63	39.035	18.202	58.826	1.00	52.56
	502 503	N CA	GLY	64	38.479	20.268	58.171	1.00	71.62
20	504	c	GLY GLY	64 64	38,243 39,138	20.690 21.809	59.528	1.00	71.62
	505	ŏ	GLY	64	39.954	22.299	59. 96 2 59.196	1.00	71.62
	506	Ň	GLU	65	38.957	22.205	61.211	1.00 1.00	71.62 87.67
	507	CA	GLU	65	39.712	23.270	61.833	1.00	87.67
05	508	CB	GLU	65	38.887	23.868	62.967	1.00	86.11
25	509	CG	GLU	65	39.602	24.889	63.834	1.00	86.11
	510	CD	GLU	65	38.934	25.056	65.194	1.00	86.11
	511 512	OE1 OE2	GLU	65	39.124	24.172	66.068	1.00	86.11
	513	C	GLU	65 65	38.210	26.059	65.386	1.00	86.11
30	514	ŏ	GLU	65	40.988 41.072	22.684 21.485	62.395 62.640	1.00	87.67
	515	Ň	TYR	66	41.980	23.539	62.598	1.00 1.00	87.67
	516	CA	TYR	66	43.258	23.129	63.151	1.00	99.15 99.15
	517	CB	TYR	66	44.246	22.786	62.044	1.00	44.24
35	518	CG	TYR	66	44.017	21.547	61.224	1.00	44.24
23	519 520	CD1	TYR	66	43.042	21.512	60.225	1.00	44.24
	520 521	CE1 CD2	TYR TYR	66 66	42.884	20.381	59.401	1.00	44.24
	522	CE2	TYR	66 66	44.838 44.700	20.429 19.299	61.399 60.600	1.00	44.24
	523	CZ	TYR	66	43.719	19.270	59. 59 6	1.00 1.00	44.24 44.24
40	524	OH	TYR	66	43.560	18.121	58.822	1.00	44.24
	525	С	TYR	66	43.848	24.303	63.935	1.00	99.15
	526	o	TYR	66	43.714	25.462	63.526	1.00	99.15
	527	N	LYS	67	44.502	23.996	65.052	1.00	76.23
45	528 529	CA CB	LYS LYS	67 67	45.158	25.008	65.883	1.00	76.23
73	530	CG	LYS	67 67	44.357 42.934	25.311	67.152	1.00	84.41
	531	CD	LYS	67	42.212	25.780 25.802	66.944 68.294	1.00	84.41
	532	CE	LYS	67	40.725	26.104	68.164	1.00 1.00	84.41 84.41
~~	533	NZ	LYS	67	40.042	25.844	69.456	1.00	84.41
50	534	Ç	LYS	67	46.477	24.393	66.303	1.00	76.23
	535	0	LYS	67	46.621	23.170	66.300	1.00	76.23
	536 537	N CA	CYS	68	47.449	25.235	66.625	1.00	101.62
	537 538	CA C	CYS	68	48.729	24.757	67.110	1.00	101.62
55	539	ŏ	CYS	68 68	49.018 48.586	25. 644 26. 79 7	68.2°3	1.00	101.62
	540	СВ	CYS	68	49.836	24.883	68.355 66.058	1.00	101.62
	541	SG	CYS	68	50.287	26.560	65.501	1.00 1.00	149.58 149.58
	542	N	GLN	69	49.716	25.099	69.281	1.00	93.84
۷0	543	CA	GLN	69	50.045	25.874	70.458	1.00	93.84
60	544	СВ	GLN	69	48.935	25.756	71.497	1.00	108.47
	545 546	CG	GLN	69	49.325	26.336	72.838	1.00	108.47
	546 547	CD OE1	GLN	69	48.228	26.198	73.866	1.00	108.47
	547 548	NE2	GLN GLN	69 60	47.421	25.266 27.446	73.801	1.00	108.47
65	549	C	GLN	69 69	48.197 51.362	27.116 25.450	74.835 74.097	1.00	108.47
	550	ŏ	GLN	69	51.813	25.450 24.310	71.087 70.919	1.00 1.00	93.84
	551	N	HIS	70	51.986	26.399	71.778	1.00	93.84 149.64
	552	CA	HIS	70	53.221	26.162	72.504	1.00	149.64
70	553	CB	HIS	70	54.272	27.216	72.161	1.00	188.52
70	554	CG	HIS	70	54.952	26.965	70.857	1.00	168.52

	555	CD2	HIS	7 0 -	54.804	25.981	69.944	1.00	188.52
	556	ND1	HIS	70	55.951	27.788	70.358	1.00	188.52
	557 550	CE1	HIS	70	58.375	27.316	69.210	1.00	188.52
5	558 559	NE2 C	HIS HIS	70 70	55.693	26.212	68.928	1.00	188.52
3	560	ŏ	HIS	70 70	52.788 52.566	26.284 27.385	73.952	1.00	149.64
	561	Ň	GLN	70 71	52.642	27.365 25.132	74.454 74.599	1.00	149.64
	562	CA	GLN	71	52.191	25.045	74.599 75.981	1.00 1.00	126.80
	563	СВ	GLN	71	52.974	23.964	76. 726	1.00	126.80 175.94
10	564	CG	GLN	71	52.367	23.589	78.072	1.00	175.94
	565	CD	GLN	71	53.119	22.461	78.752	1.00	175.94
	566	OE1	GLN	71	54.130	21.984	78.241	1.00	175.94
	567	NE2	GLN	71	52.631	22.031	79. 909	1.00	175.94
15	568 569	C O	GLN GLN	71 74	52.267	26.359	76.745	1.00	126.80
13	570	N	GLN	71 72	53.343 51.096	26.934	76.927	1.00	126.80
	571	CA	GLN	72	50.936	26.825 28.060	77.169 77.933	1.00	138.09
	572	СВ	GLN	72	51.762	28.017	79.214	1.00 1.00	138.09
	573	CG	GLN	72	51.264	27.031	80.242	1.00	197.82 197.82
20	574	CD	GLN	72	49.767	27.138	80.538	1.00	197.82
	575	OE1	GLN	72	49.158	28.202	80.397	1.00	197.82
	576	NE2	GLN	72	49.175	26.028	80.973	1.00	197.82
	577	C	GLN	72	51.252	29.347	77.196	1.00	138.09
25	578 579	0 N	GLN VAL	72 70	51.503	30.377	77.821	1.00	138.09
23	580	ČA	VAL	73 73	51.243 51.505	29.291	75.871	1.00	127.03
	581	CB	VAL	73 73	52.817	30.477 30.340	75.070	1.00	127.03
	582	CG1	VAL	73	53.197	31.683	74.250 73.626	1.00	90.79
	583	CG2	VAL	73	53.943	29.826	75.148	1.00 1.00	90.79
30	584	С	VAL	73	50.314	30.625	74.134	1.00	90.79 127.03
	585	0	VAL	73	50.467	30.866	72.936	1.00	127.03
	586	N	ASN	74	49.119	30.457	74.693	1.00	129.72
	587 588	CA	ASN	74	47.890	30.577	73.920	1.00	129.72
35	589	CB CG	ASN ASN	74 74	47.721	31.993	73.390	1.00	137.31
75	590	OD1	ASN	74 74	47.576 48.512	33.011 33.785	74.476	1.00	137.31
	591	ND2	ASN	74	46.400	33.015	74.713 75.123	1.00	137.31
	592	C	ASN	74	47.820	29.655	72.709	1.00 1.00	137.31 129.72
40	593	0	ASN	74	48.836	29.209	72.176	1.00	129.72
40	594	N	GLU	75	46.600	29.404	72.254	1.00	128.29
	595	CA	GLU	75	46.377	28.580	71.080	1.00	128.29
	596	CB	GLU	.75	44.998	27.934	71.175	1.00	132.07
	597 598	CG CD	GLU	75 75	44.672	27.459	72.584	1.00	132.07
45	599	OE1	GLU	75 75	43.266 42.439	26.922 27.252	72.700	1.00	132.07
	600	OE2	GLU	75 75	42.989	26.185	71.821 73.673	1.00	132.07
	601	c	GLU	75	46.446	29.547	73.873 69.897	1.00 1.00	132.07
	602	0	GLU	75	46.432	30.757	70.089	1.00	128.29 128.29
50	603	N	SER	76	48.545	29.033	68.681	1.00	77,19
50	604	CA	SER	76	46.595	29.901	67.506	1.00	77.19
	605	CB	SER	76	47.321	29.207	66.363	1.00	54.46
	606 607	og .	SER	76	46.418	28.351	65.649	1.00	54.46
	608	C	SER SER	76 76	45.175	30.169	67.033	1.00	77.19
55 ·	609	N	GLU	76 77	44.208 45.038	29.659	67.603	1.00	77.19
	610	CA	GLU	77	43.711	30.966 31.198	65.983 65.444	1.00	74.40
	611	CB	GLU	77	43.652	32,492	64.632	1.00 1.00	74.40 153.94
	612	CG	GLU	77	43.693	33.746	65.491	1.00	153.94
60	613	CD	GLU	77	42.624	33.749	66.578	1.00	153.94
60	614	OE1	GLU	77	41.418	33.712	66.237	1.00	153.94
	615	OE2	GLU	77	42.992	33.787	67.775	1.00	153.94
	616 617	C	GLU	77	43.460	29.998	64.558	1.00	74.40
	618	0 N	GLU PRO	77 79	44.375	29.495	63.913	1.00	74.40
65	619	CD	PRO	78 78	42.215 41.068	29.512	64.527	1.00	88.95
	620	CA	PRO	78	41.857	29.938 28.352	65.344	1.00	122.79
	621	CB	PRO	78	40.385	28.138	63.712 64.046	1.00 1.00	88.95
	622	CG	PRO	78	40.268	28.670	65.428	1.00	122.79 122.79
70	623	Ç	PRO	78	42.061	28.542	62.221	1.00	88.95
70	624	0	PRO	78	41.901	29.640	61.688	1.00	88.95
								· -	

	625	N	VAL	79	42.415	27.447	61.560	1.00	101.27
	626	CA CB	VAL	79	42.604	27.427	60.119	1.00	101.27
	627 628	CG1	VAL VAL	79 79	44.042 44.177	27.114	59.735	1.00	79.48
Š	629	CG2	VAL	79	44.962	27.097 28.130	58.226 60.341	1.00 1.00	79.48
_	630	C	VAL	79	41.727	26.304	59.592	1.00	79.48 101.27
	631	0	VAL	79	41.846	25.155	60.025	1.00	101.27
	632	N	TYR	80	40.851	26.629	58.655	1.00	55.37
10	633	CA	TYR	80	39.973	25.618	58.115	1.00	55.37
10	634 635	CB CG	TYR TYR	80 80	38.551	26.145	58.016	1.00	122.28
	636	CD1	TYR	80	38.004 38.278	26.497 27. 73 3	59 .364 59. 942	1.00 1.00	122.28
	637	CE1	TYR	80	37.817	28.049	61.208	1.00	122.28 122.28
	638	CD2	TYR	80	37.250	25.577	60.088	1.00	122.28
15	639	CE2	TYR	80	36.782	25.877	61.357	1.00	122.28
	640 641	CZ OH	TYR	80	37.069	27.117	61.915	1.00	122.28
	642	C	TYR TYR	80 80	36.615 40.390	27.424 25.066	63.180	1.00	122.28
	643	ŏ	TYR	80	40.474	25.780	56.779 55.795	1.00 1.00	55.37 55.37
20	644	N	LEU	81	40,627	23.768	56.765	1.00	67.93
	645	CA	LEU	81	41.026	23.065	55.578	1.00	67.93
	646	CB	LEU	81	42.016	22.014	55.982	1.00	70.09
	647 648	CG CD1	LEU LEU	81 81	42.558 43.387	21.223 22.150	.54.819	1.00	70.09
25	649	CD2	LEU	81	43.411	20.066	53.967 55.338	1.00 1.00	70.09
	650	C	LEU	81	39 791	22.405	55.006	1.00	70.09 67.93
	651	0	LEU	81	38.856	22.098	55.763	1.00	67.93
	652	N	GLU	82	39.732	22.188	53.691	1.00	70.25
30	653 654	CA CB	GLU GLU	82 82	38.569 37.486	21.530 22.562	53.079	1.00	70.25
-	655	CG	GLU	82	36.199	22.902 21.935	52.737 52.234	1.00 1.00	131.12 131.12
	656	CD	GLU	82	34.994	22.847	52.359	1.00	131.12
	657	OE1	GLU	82	35.091	24.023	51.958	1.00	131.12
35	658 659	OE2 C	GLU GLU	82 82	33.940	22.384	52.847	1.00	131.12
33	660	ŏ	GLU	82	38.957 39.425	20.709 21.261	51.843 50.850	1.00 1.00	70.25 70.25
	661	N	VAL	83	38.769	19.386	51.918	1.00	70.25 52.36
	662	CA	VAL	83	39.106	18.469	50.815	1.00	52.36
40	663 664	CB CG1	VAL	83	39.452	17.094	51.350	1.00	43.44
40	665	CG2	VAL VAL	83 83	40. 082 40.359	16.245 17.241	50.244 52.544	1.00 1.00	43.44
	666	c	VAL	83	37.995	18.302	49.768	1.00	43.44 52.36
	667	0	VAL	83	36.852	18.022	50.105	1.00	52.36
45	668	N	PHE	84	38.342	18.479	48.498	1.00	63.83
45	669 670	CA CB	PHE PHE	84 84	37.368 37.359	18.369	47.426	1.00	63.83
	671	ČĠ	PHE	84	36.918	19.633 20.841	46.562 47.294	1.00 1.00	62.38 62.38
	672	CD1	PHE	84	37.692	21.345	48.329	1.00	62.38
50	673	CD2	PHE	84	35.680	21.429	47.020	1.00	62.38
20	674 675	CE1 CE2	PHE	84	37.244	22.418	49.092	1.00	62.38
	676	CZ	PHE PHE	84 84	35.223 36.007	22.506 22,998	47.780	1.00	62.38
	677	č	PHE	84	37.606	17.175	48.823 46.527	1.00 1.00	61.83 63.83
	678	0	PHE	84	38.619	16.477	46.630	1.00	63.83
55	679	N	SER	85	36.635	16.952	45.650	1.00	70 <u>.2</u> 2
	680 681	CA CB	SER SER	85 85	36. 663	15.891	44.671	1.00	70.22
	682	OG OD	SER	85	36.006 36.099	14.615 13.567	45.197 44.235	1.00 1.00	107.∔2 107.42
	683	C	SER	85	35. 83 3	16.465	43.552	1.00	70.22
60	684	0	SER	85	34.608	16.501	43.625	1.00	70.22
	685 686	N CA	ASP ASP	86 86	36.513	16.953	42.528	1.00	30.45
	687	CB	ASP	86 86	35.835 35.151	17.517 18. 79 6	41.391 41. 79 9	1.00	30.45
,-	688	CG	ASP	86	34.005	19.121	40.908	1.00 1.00	66.75 66.75
65	689	OD1	ASP	86	34.186	19.182	39.664	1.00	66.75
	690 691	OD2	ASP	86	32.909	19.311	41.455	1.00	68.75
	692	C O	ASP ASP	8 6 86	36.876 38.074	17.768 17.603	40.303	1.00	30.45
	693	Ň	TRP	87	36.427	17.603 18.122	40.551 39.101	1.00 1.00	30.45 54.88
70	694	CA	TRP	87	37.329	18.392	37.986	1.00	54.88

	695	CB	TRP	87	36.541	18.398	36.686	1.00	120.63
	696	CG.	TRP	87	36.228	17.051	36.187	1.00	120.63
	697 698	CD2 CE2	TRP TRP	87 87	35.123	16.242	38.559	1.00	120.63
5	699	CE3	TRP	87 87	35.205 34.043	15.040 16.411	35.822 37.446	1.00	120.63
	700	CD1	TRP	87	36.936	16.335	35.269	1.00 1.00	120.63
	701	NE1	TRP	87	36.336	15.125	35.036	1.00	120.63 120.63
	702	CZ2	TRP	87	34.277	14.011	35.939	1.00	120.63
10	703 704	CZ3 CH2	TRP TRP	87 87	33.109 33.231	15.387	37.568	1.00	120.63
	705	C	TRP	87	38.051	14.202 19.726	36.813 38.150	1.00 1.00	120.63
	706	0	TRP	87	39.248	19.818	37.884	1.00	54.88 54.88
	707	N	LEU	88	37.307	20.751	38.578	1.00	42.94
15	708 709	CA CB	LEU	88	37.831	22.113	38.806	1.00	42.94
13	710	CG	LEU	88 88	37.131 37.526	23.157 23.193	37. 946	1.00	57.40
	711	CD1	LEU	88	36.761	24.330	36.485 35.822	1.00 1.00	57.40 57.40
	712	CD2	LEU	88	39.030	23.370	36. 354	1.00	57.40 57.40
20	713	C	LEU	88	37.671	22.549	40.235	1.00	42.94
20	714 715	0 N	LEU	88 89	36.666	22.301	40.870	1.00	42.94
	716	CA	LEU	89	38.681 38.667	23.225 23.700	40.733	1.00	58.27
	717	СВ	LEU	89	39.556	22.835	42.085 42.951	1.00 1.00	58.27 5.00
25	718	CG	LEU	89	39.739	23.331	44.403	1.00	5.00
23	719 720	CD1 CD2	LEU	89	38.371	23.632	45.112	1.00	5.00
	720 721	C	LEU	89 89	40.628 39.237	22.281 25.082	45.195	1.00	5.00
	722	ŏ	LEU	89	40.346	25.062 25.279	42.056 41.555	1.00 1.00	58.27
20	723	N	LEU	90	38.486	26.043	42.582	1.00	58.27 24.40
30	724	CA	LEU	90	38.995	27.407	42.636	1.00	24.40
	725 726	CB CG	LEU	90	37.861	28.425	42.585	1.00	63.96
	727	CD1	LEU	90 90	38.331 39.284	29.867 30.173	42.711	1.00	63.96
	728	CD2	LEU	90	37.134	30.803	41.570 42.692	1.00 1.00	63.96 63.96
35	729	C	LEU	90	39.702	27.535	43.969	1.00	24.40
	730 731	O N	LEU GLN	90	39.057	27.496	45.000	1.00	24.40
	732	CA	GLN	91 91	41.017 41.721	27.690 27.825	43.970	1.00	52.44
	733	CB	GLN	91	43.018	27.058	45. 23 4 45.151	1.00 1.00	52.44 32.27
40	734	ÇG	GLN	91	42.820	25.718	44.534	1.00	32.27
	735 736	CD	GLN	91	44.020	24.841	44.727	1.00	32.27
	736 737	OE1 NE2	GLN GLN	91 91	45.010 43. 9 62	24.901	43.957	1.00	32.27
	738	C	GLN	91	43.902	24.016 29.299	45.788 45.554	1.00 1.00	32.27
45	739	0	GLN	91	42.060	30.142	44.657	1.00	52.44 52.44
	740	N	ALA	92	42.075	29.633	46.831	1.00	55.47
	741 742	CA CB	ALA ALA	92	42.345	31.018	47.175	1.00	55.47
	743	Č.	ALA	92 92	41.076 43.381	31.735 31.100	47.638	1.00	37.36
50	744	0	ALA	92	43.384	30.316	48.246 49.183	1.00 1.00	55.47 55.47
	745	N	SER	93	44.263	32.064	48.077	1.00	51.36
	748 747	CA CB	SER	93	45.329	32.345	49.008	1.00	51.36
	748	OG OG	SER SER	93 93	45.997 45.009	33.647	48.583	1.00	54.66
55	749	č	SER	93	44.690	34.650 32.509	48.346 50.378	1.00 1.00	54.66 51.36
	750	0	SER	93	45.238	32.104	51.395	1.00	51.36
	751 750	N	ALA	94	43.521	33.124	50.397	1.00	46.22
	752 753	· CA CB	ALA ALA	94 94	42.822	33.313	51.645	1.00	46.22
60	754	Č	ALA	94	43.522 41.393	34.352 33.723	52.496 51.340	1.00	74.92
	755	Ö	ALA	94	41.111	34.357	50.317	1.00 1.00	46.22 46.22
	756	N	GLU	95	40.489	33.326	52.231	1.00	89.58
	757 758	CA	GLU	95 05	39.074	33.605	52.065	1.00	89.58
65	759	CB CG	GLU	95 95	38.283 38.549	32.448	52.662	1.00	145.77
	760	CD	GLU	95	37.950	31.139 29.953	51.938 52.650	1.00	145.77
	761	OE1	GLU	95	38.060	28.826	52.118	1.00 1.00	145.77 145.77
	762 763	OE2	GLU	95	37.373	30.145	53.742	1.00	145.77
70	763 764	C O	GLU	95 95	38.662	34.938	52.678	1.00	89.58
		•	~~~	83	37.661	35.546	52. 28 9	1.00	89.58

	765 766	N CA	VAL VAL	96 [.]	39.453 39.233	35.379 36.643	53.644 54.322	1.00	75.49 75.49
	767	CB:	VAL	96	38.995	36.436	55.819	1.00	87.57
5	768	CG1	VAL	96	38.710	37.771	56. 480	1.00	87.57
)	769	CG2	VAL	96	37.847	35.467	56.032	1.00	87.57
	770 771	C	VAL	96 96	40.537	37.402	54.128	1.00	75.49
	772	N	VAL VAL	96 97	41.578 40.482	37.016 38.474	54.665	1.00	75.49
	773	CA	VAL	97	41.670	38.471 39.254	53.345 53.066	1.00	96.50
10	774	CB	VAL	97	41.929	39.335	51.553	1.00 1.00	96.50
	775	CG1	VAL	97	42.920	40.443	51.259	1.00	66.57 66.57
	776	CG2	VAL	97	42.472	38.004	51.049	1.00	66.57
	777	С	VAL	97	41.598	40.665	53.613	1.00	96.50
15	778	0	VAL	97	40.583	41.352	€3.473	1.00	96.50
15	779	N	MET	98	42.693	41.088	∍4. 23 7	1.00	97.55
	780 781	CA CB	MET	98	42.784	42.425	€ 4.799	1.00	97.55
	782	CG	MET MET	98 98	43.870	42.482	55.887	1.00	148.78
	783	SD	MET	98	43.567 44.803	41.601 41.635	57.108 58.454	1.00	148.78
20	784	CE	MET	98	45.665	40.108	58.454 58.182	1.00 1.00	148.78
	785	С	MET	98	43.098	43.411	53.682	1.00	148.78 97.55
	786	0	MET	98	44.143	43.318	53.034	1.00	97.55
	787	N	GLU	99	42.161	44.329	53.455	1.00	85.18
25	788	CA	GLU	99	42.265	45.380	52.450	1.00	85.18
23	789	CB	GLU	99	41.565	46.635	52.988	1.00	186.55
	790 791	CD	GLU	99	41.620	47.868	52.109	1.00	186.55
	792	OE1	GLU	99 9 9	40.716 40.827	48.978 49.337	52.629	1.00	186.55
	793	OE2	GLU	99	39.894	49.490	53.823	1.00	186.55
30	794	č	GLU	99	43.724	45.677	51.839 52.137	1.00 1.00	186.55
	795	0	GLU	99	44.605	45.506	52.990	1.00	85.18 85.18
	796	N	GLY	100	43.991	46.106	50.909	1.00	64.51
	797	CA	GLY	100	45.362	46.432	50.549	1.00	64.51
35	798	C	GLY	100	46.371	45.293	50.459	1.00	64.51
JJ	799 800	0 N	GLY GLN	100	47.508	45.528	50.054	1.00	64.51
	801	CA	GLN	101 101	45.987 46.896	44.075 42.930	50.839	1.00	91.02
	802	CB	GLN	101	46.631	41.933	50.742 51.875	1.00 1.00	91.02
	803	CG	GLN	101	47.181	42.383	53.207	1.00	93.41 93.41
40	804	CD	GLN	101	48.671	42.663	53.133	1.00	93.41
	805	OE1	GLN	101	49.117	43.530	52.384	1.00	93.41
	806	NE2	GLN	101	49.448	41.926	53.906	1.00	93.41
	807	C	GLN	101	46.716	42,260	49.373	1.00	91.02
45	808 809	O N	GLN	101	45.909	42.712	48.567	1.00	91.02
73	810	CD	PRO PRO	102 102	47.484 48.769	41.195	49.078	1.00	67.73
	811	CA	PRO	102	47.324	40.802 40.547	49.675 47.778	1.00	29.55
	812	CB	PRO	102	48.730	40.145	47.432	1.00 1.00	67.73 29.55
	813	CG	PRO	102	49.248	39.718	48.721	1.00	29.55
50	814	С	PRO	102	46.398	39.353	47.784	1.00	67.73
	815	0	PRO	102	46.385	38.564	48.719	1.00	67.73
	816	N	LEU	103	45.636	39.227	46.707	1.00	40.45
	817 818	CA	LEU	103	44.688	38.154	46.552	1.00	40.45
55	819	CB CQ	LEU LEU	103 103	43.308	38.743	46.277	1.00	52.62
-	820	CD1	LEU	103	42.141 42.345	37.774 36.942	46.464 47.721	1.00	52.62
	821	CD2	LEU	103	40.852	38.574	46.533	1.00 1.00	52
	822	C	LEU	103	45.115	37.227	45.415	1.00	52.62 40.45
	823	0	LEU	103	45.314	37.665	44.280	1.00	40.45
60	824	N	PHE	104	45.274	35.945	45.739	1.00	56.34
	825	CA	PHE	104	45.680	34.942	44.762	1.00	56.34
	826	CB	PHE	104	46.898	34.159	45.251	1.00	133.82
	827 828	CG CD1	PHE	104	48.053	35.016	45.592	1.00	133.82
65	829	CD2	PHE	104 104	48.298 48.870	35.367 35.539	46.905	1.00	133.82
	830	CE1	PHE	104	48.870 49.344	35.528 36.223	44.594 47.229	1.00	133.82
	831	CE2	PHE	104	49.924	36.389	47.229 44.906	1.00 1.00	133.82 133.82
	832	CZ	PHE	104	50.161	36.738	46.224	1.00	133.82
70	833	Ç	PHE	104	44.570	33.958	44.477	1.00	56.34
70	834	0	PHE	104	43.923	33.468	45.388	1.00	56.34

	835	N	LEU	105	44.363	33.668	43.202	1.00	51.84
	836	CA	LEU	105	43.341	32.730	42.792	1.00	51.84
	837 838	CB CG	LEU	105	42.199	33.440	42.086	1.00	27.36
5	839	CD1	LEU	105 105	41.385 40.132	34.348 34.710	42.989	1.00	27.36
•	840	CD2	LEU	105	40.988	33.638	42.214 44.293	1.00 1.00	27.36
	841	C	LEU	105	43.897	31.690	41.857	1.00	27.36 51.84
	842	0	LEU	105	44.802	31.948	41.068	1.00	51.84
10	843 844	N CA	ARG	106	43.337	30.499	41.929	1.00	60.02
10	845	CB	ARG ARG	106 106	43.820 44.949	29.474 28.740	41.063	1.00	60.02
	846	ĊĠ	ARG	106	45.476	27.618	41.722 40.886	1.00 1.00	28.53
	847	CD	ARG	106	46.314	26.830	41.814	1.00	28.53 28.53
15	848	NE	ARG	106	47.260	25.934	41.174	1.00	28.53
13	849 850	CZ NH1	ARG ARG	106 106	47.904	25.010	41.864	1.00	28.53
	851	NH2	ARG	106	47.633 48.819	24.925 24.231	43.173 41.267	1.00	28.53
	852	C	ARG	106	42.775	28.496	40.663	1.00 1.00	28.53 60.02
20	853	0	ARG	106	42.121	27.884	41.498	1.00	60.02
20	854	N	CYS	107	42.625	28.378	39.353	1.00	30.47
	855 856	CA C	CYS CYS	107 107	41.692	27.449	38.763	1.00	30.47
	857	ŏ	CYS	107	42.484 43.098	26.168 25.892	38. 6 45 37. 60 7	1.00	30.47
	858	СВ	CYS	107	41.261	27.937	37. 3 98	1.00 1.00	30.47 52.55
25	859	SG	CYS	107	39.630	27.258	36.984	1.00	52.55
	860 861	N CA	HIS	108	42.476	25.399	39.733	1.00	44.34
	862	CB	HIS HIS	108 108	43.224	24.162	39.808	1.00	44.34
	863	ČG	HIS	108	43.644 44.610	23.916 22.800	41.229 41.351	1.00 1.00	41.81
30	864	CD2	HIS	108	44.648	21.734	42.178	1.00	41.81 41.81
	865	ND1	HIS	108	45.701	22.686	40.519	1.00	41.81
	866 867	CE1 NE2	HIS HIS	108	46.370	21.595	40.832	1.00	41.81
	868	C	HIS	108 108	45.753 42.526	20.999 22.934	41.835	1.00	41.81
35	869	ŏ	HIS	108	41.515	22.530	39. 31 0 39. 83 8	1.00 1.00	44.34 44.34
	870	Ņ	GLY	109	43.084	22.315	38.293	1.00	45.07
	871	CA	GLY	109	42.461	21.121	37.772	1.00	45.07
	872 873	C	GLY GLY	109	42.909	19.890	38.534	1.00	45.07
40	874	Ň	TRP	109 110	44.015 42.026	19.831 18.902	39.097 38.5 6 5	1.00	45.07
	875	CA	TRP	110	42.293	17.641	39.239	1.00 1.00	46.18 46.18
	876	СВ	TRP	110	41.156	16.653	38.932	1.00	36.88
	877 878	CG	TRP	110	41.347	15.329	39.576	1.00	36.88
45	879	CD2 CE2	TRP TRP	110 110	41.040 41.526	15.001	40.923	1.00	36.88
	880	CE3	TRP	110	40.388	13.697 15.690	41.176 41.973	1.00 1.00	36.88 36.88
	881	CD1	TRP	110	41.989	14.231	39.047	1.00	36.88
	882	NE1	TRP	110	42.110	13.251	39.999	1.00	36.88
50	883 884	CZ2 CZ3	TRP TRP	110	41.408	13.055	42.401	1.00	36.88
50	885	CH2	TRP	110 110	40.264 40.773	15.061 13.748	43.204	1.00	36.88
	886	Ċ _	TRP	110	43.615	17.100	43.408 38.726	1.00 1.00	36.88
	887	0	TRP	110	43.910	17.235	37.539	1.00	46.18 46.18
55	888	N	ARG	111	44.416	16.510	39.609	1.00	63.08
JJ	889 890	CA CB	ARG	111	45.704	15.952	39.200	1.00	63.08
	891	cc	ARG	111 111	45.488 44.790	14.690 13.594	38.373	1.00	97.86
	892	CD	ARG	111	45.652	13.108	39.132 40.265	1.00 1.00	97.96 97.96
~	893	NE	ARG	111	48.850	12.447	39.758	1.00	97.96
60	894	CZ	ARG	111	47.845	12.019	40.528	1.00	97.96
	895 896	NH1 NH2	ARG	111	47.785	12.190	41.846	1.00	97.96
	897	C	ARG ARG	111 111	48.894 46.465	11.413	39.982	1.00	97.96
	898	ŏ	ARG	111	47.152	16.961 16.596	38.358 37.406	1.00 1.00	63.08 63.08
65	899	N	ASN	112	46.324	18.237	38.685	1.00	111.35
	900	CA	ASN	112	47.011	19.247	37.914	1.00	111.35
	901 902	CB CG	ASN	112	48.500	19.213	38.245	1.00	81.63
	903	OD1	ASN ASN	112 112	48.814 48.719	19.880	39.568	1.00	81.63
70	904	ND2	ASN	112	49.182	21.101 19.082	39.701 40.556	1.00	81.63
				· · · · · ·			70.000	1.00	81.63

	905 906	c o	ASN ASN	112 112	46.791 47.744	18.987 18.946	36.424 35.648	1.00 1.00	111.35
	907	N ·	TRP	113	45.540	18.783	36.027	1.00	111.35 91.49
5	908	CA	TRP	113	45.258	18.560	34.623	1.00	91.49
J	909	CB	TRP	113	43.894	17.929	34.393	1.00	88.74
	910 911	CG CD2	TRP TRP	113	43.813	16.506	34.706	1.00	88.74
	912	CE2	TRP	113 113	42.611 42.998	15.767	34.927	1.00	88.74
	913	CE3	TRP	113	41.258	14.439 16.105	35.200	1.00	88.74
10	914	CD1	TRP	113	44.845	15.625	34.927 34.837	1.00	88.74
	915	NE1	TRP	113	44.354	14.376	35.137	1.00 1.00	88.74
	916	CZ2	TRP	113	42.063	13.451	35.465	1.00	88.74 88.74
	917	CZ3	TRP	113	40.338	15.124	35.188	1.00	88.74
15	918	CH2	TRP	113	40.742	13.810	35.459	1.00	88.74
15	919	C	TRP	113	45.255	19.871	33.895	1.00	91.49
	920 921	O N	TRP	113	44.941	20.922	34.463	1.00	91.49
	922	CA	ASP ASP	114	45.567	19.780	32.611	1.00	60.02
	923	CB	ASP	114 114	45.599 46.201	20.940	31.755	1.00	60.02
20	924	ĊĠ	ASP	114	47.637	20.569 20.066	30.390	1.00	89.00
	925	OD1	ASP	114	48.360	20.492	30.498 31.430	1.00 1.00	89.00
	926	OD2	ASP	114	48.053	19.254	29.643	1.00	89.00
	927	С	ASP	114	44.210	21.555	31.585	1.00	89.00 60.02
25	928	0	ASP	114	43.248	20.897	31.224	1.00	60.02
23	929	N	VAL	115	44.104	22.832	31.879	1.00	103.64
	930 931	CA	VAL	115	42.836	23.482	31.712	1.00	103.64
	932	CB CG1	VAL VAL	115	42.283	23.916	33.063	1.00	73.31
	933	CG2	VAL	115	40.951	24.620	32.902	1.00	73.31
30	934	C	VAL	115 . 115	42.153 43.127	22.682 24.647	33.943	1.00	73.31
	935	ŏ	VAL	115	43.127 44.162	24.047 25.304	30.805	1.00	103.64
	936	Ň	TYR	116	42.232	24.861	30.904 29.868	1.00 1.00	103.64
	937	CA	TYR	116	42.415	25.932	28.943	1.00	59.95 59.95
25	938	CB	TYR	116	42.503	25.377	27.529	1.00	98.72
35	939	CG	TYR	116	43.712	24.492	27.362	1.00	98.72
	940	CD1	TYR	116	43.675	23.152	27.726	1.00	98.72
	941 942	CE1 CD2	TYR TYR	116	44.815	22.360	27.650	1.00	98.72
	943	CE2	TYR	116 116	44.922	25.017	26.914	1.00	98.72
40	944	cz	TYR	116	46.067 46.008	24.233 22.908	26.839	1.00	98.72
	945	OH	TYR	116	47.147	22.132	27.207 27.144	1.00	98.72
	946	C	TYR	116	41.271	26.898	29.083	1.00 1.00	98.72 59.95
	947	. 0	TYR	116	40,499	26.821	30.047	1.00	59.95
15	948	N	LYS	117	41.176	27.814	28.127	1.00	66.79
45	949	CA	LYS	117	40.132	28.813	28.132	1.00	66.79
	950 951	CB CG	LYS	117	38.946	28.332	27.295	1.00	151.68
	952	CD	LYS LYS	117 117	37.902	29.406	27.008	1.00	151.68
	953	CE	LYS	117	38.475 37.451	30.515 31.604	26.129	1.00	151.68
50	954	NZ	LYS	117	38.062	32.685	25.848 25.034	1.00	151.68
	955	C	LYS	117	39.676	29.122	29.559	1.00 1.00	151.68
	956	0	LYS	117	38.472	29.233	29.810	1.00	66.79 66.79
	957	N	VAL	118	40.622	29.256	30.495	1.00	43.61
55	958	CA	VAL	118	40.243	29.564	31.879	1.00	43.61
55	959 960	CB CG1	VAL	118	41.429	29.461	32.852	1.00	34.30
	961	CG2	VAL	118	40.912	29.485	34.289	1.00	34.30
	962	C	VAL VAL	118 118	42.246	28.215	32.562	1.00	34.30
	963	ŏ	VAL	118	39.657 40.002	30.977 31.881	31.998	1.00	43.61
60	964	Ñ	ILE	119	38.772	31.168	31.235 32.963	1.00	43.61
	965	CA	ILE	119	38.135	32.458	33.140	1.00 1.00	47.57 47.57
	966	CB	ILE	119	36.895	32.621	32.203	1.00	47.57 48.87
	967	CG2	ILE	119	36.185	33.914	32.512	1.00	48.87
65	968	CG1	ILE	119	37.317	32.657	30.730	1.00	48.87
UJ.	969 970	CD1	ILE	119	36.187	33.009	29.752	1.00	48.87
	970 971	C	ILE	119	37.651	32.620	34.567	1.00	47.57
	972	N	ILE TYR	119 120	36.846 38.125	31.827	35.052	1.00	47.57
	973	CA	TYR	120	38.125 37.647	33.645 33.835	35.256	1.00	51.27
70	974	CB	TYR	120	38.727	34.342	36.608 37.510	1.00	51.27
							07.010	1.00	24.86

	975 976	CG CD1	TYR TYR	120 120	39.921 40.823	33.471 33.174	37.546	1.00	24.86
	977	CE1	TYR	120	41.794	33.174 32.429	36.393 36.448	1.00	24.86
_	978	CD2	TYR	120	40.397	33.004	38.754	1.00 1.00	24.86
5	979	CE2	TYR	120	41.562	32.258	38.832	1.00	24.86 24.86
	980	CZ	TYR	120	42.260	31.972	37.681	1.00	24.86
	981	ŎН	TYR	120	43.423	31.233	37.816	1.00	24.86
	982 983	C	TYR	120	36.531	34.832	36.621	1.00	51.27
10	984	N	TYR TYR	120	36.486	35.751	35.802	1.00	51.27
10	985	CA	TYR	121 121	35.645 34.506	34.659 35.530	37.584	1.00	57.39
	986	CB	TYR	121	33.215	34.815	37.701 37.266	1.00	57.39
	987	CG	TYR	121	33.180	34.361	35.836	1.00 1.00	81.52 81.52
٠, -	988	CD1	TYR	121	33.923	33.263	35.423	1.00	81.52
15	989	CE1	TYR	121	33.918	32.846	34.105	1.00	81.52
	990	CD2	TYR	121	32.419	35.042	34.889	1.00	81.52
	991 992	CE2 CZ	TYR	121	32.407	34.642	33.554	1.00	81.52
	993	OH	TYR TYR	121 121	33.163 33.195	33.537 33.117	33.171	1.00	81.52
20	994	Č.	TYR	121	34.315	35.966	31.859 39.124	1.00	81.52
	995	Ó	TYR	121	34.522	35.184	40.054	1.00 1.00	57.39
	996	N	LYS	122	33.907	37.218	39.282	1.00	57.39 81.15
	997	CA	LYS	122	33.595	37.748	40.589	1.00	81.15
25	998	CB	LYS	122	34.433	38.961	40.948	1.00	110.18
23	999 1000	CD	LYS LYS	122	34.253	39.334	42.403	1.00	110.18
	1000	CE	LYS	122 122	34.827 33.834	40.684 41.772	42.722	1.00	110.18
	1002	NZ	LYS	122	34.358	43.095	42.392 42.796	1.00	110.18
	1003	C	LYS	122	32.159	38.177	42.786 40. 444	1.00 1.00	110.18 81.15
30	1004	0	LYS	122	31.834	39.050	39.642	1.00	81.15
	1005	N	ASP	123	31.289	37.539	41.209	1.00	100.05
	1006 1007	CA	ASP	123	29.875	37.861	41.159	1.00	100.05
	1007	CB CG	ASP ASP	123	29.640	39.238	41.781	1.00	124.27
35	1009	OD1	ASP	123 123	30.336 30.145	39.380 38.499	43.124	1.00	124.27
	1010	OD2	ASP	123	31.075	40.370	43.991 43.309	1.00 1.00	124.27
	1011	C	ASP	123	29.401	37.816	39.720	1.00	124.27 100.05
	1012	0	ASP	123	29.086	38.844	39.125	1.00	100.05
40	1013	N	GLY	124	29.407	36.612	39.157	1.00	103.70
40	1014 1015	CA	GLY	124	28.929	36.423	37.803	1.00	103.70
	1015	CO	GLY GLY	124 124	29.750	37.084	36.729	1.00	103.70
	1017	Ň	GLU	125	29. 983 30. 23 1	36.517 38.285	35.684 37.011	1.00	103,70
	1018	CA	GLU	125	31.033	39.025	36.046	1.00 1.00	86.80 86.80
45	1019	CB	GLU	125	30.929	40.506	36.309	1.00	167.98
	1020	CG	GLU	125	29.523	41.030	36.184	1.00	167.98
	1021 1022	CD	GLU	125	29.407	42.485	36.603	1.00	167.98
	1022	OE1 OE2	GLU GLU	125	30.209	43.326	36.133	1.00	167.98
50	1024	C	GLU	125 125	28.505 32.515	42.791 38.651	37.413	1.00	167.98
	1025	ŏ	GLU	125	33.206	38.440	35.940 36.952	1.00 1.00	86.80
	1026	N	ALA	126	33.003	38.614	34.700	1.00	86.80 117.82
	1027	CA	ALA	126	34.395	38.279	34.411	1.00	117.82
55	1028	СВ	ALA	126	34.627	38.310	32.891	1.00	16.51
23	1029 1030	C	ALA	126	35.399	39.201	35.101	1.00	117.82
	1031	O N	ALA LEU	126	35.141	40.384	35.284	1.00	117.82
	1032	CA	LEU	127 127	36.556 37.572	38.665 39.490	35.467	1.00	95.95
	1033	CB	LEU	127	38.604	38.639	36.104 36.840	1.00 1.00	95.95 46.01
60	1034	CG	LEU	127	38.205	37.916	38.119	1.00	46.01
	1035	CD1	LEU	127	39.484	37.355	38.754	1.00	46.01
	1036	CD2	LEU	127	37.491	38.848	39.082	1.00	46.01
	1037 1038	CO	LEU	127	38.281	40.327	35.050	1.00	95.95
65	1039	N	LEU LYS	127	38.475	39.885	33.911	1.00	95.95
	1040	CA	LYS	128 128	38.664 39.342	41.538 42.486	35.450	1.00	158.42
	1041	СВ	LYS	128	39.220	42.400 43.899	34.573 35.142	1.00	158.42
	1042	CG	LYS	128	37.787	44.386	35.312	1.00 1.00	155.76 155.76
70	1043	CD	LYS	128	37.114	44.590	33.960	1.00	155.76
70	1044	CE	LYS	128	35.689	45.116	34.097	1.00	155.76

	1045	NZ	LYS	128	35,067	45.392	20.700	4.00	
	1046	C	LYS	128	40.813	45.392 42.148	32.766	1.00	155.76
	1047	ŏ	LYS				34.369	1.00	158.42
	1048	Ň	TYR	128	41.144	41.178	33.693	1.00	158.42
5	1049			129	41.698	42.949	34.954	1.00	117.79
5		CA	TYR	129	43.132	42.714	34.800	1.00	117.79
	1050	CB	TYR	129	43.851	43.967	34.297	1.00	165.79
	1051	CG	TYR	129	43.199	44.664	33.137	1.00	165.79
	1052	CD1	TYR	129	42.151	45. 563	33.344	1.00	165.79
	1053	CE1	TYR	129	41.561	46.234	32.280	1.00	165.79
10	1054	CD2	TYR	129	43.643	44.447	31.832	1.00	165.79
	1055	CE2	TYR	129	43.060	45.112	30.759	1.00	165.79
	1056	CZ	TYR	129	42.022	46.005	30.991	1.00	165.79
	1057	OH	TYR	129	41.451	46.671	29.932	1.00	165.79
	1058	С	TYR	129	43.834	42.279	36.077	1.00	
15	1059	Ó	TYR	129	44.261	43.117	36.875	1.00	117.79
	1060	Ň	TRP	130	43.956	40.972	36.267		117.79
	1061	CA	TRP	130	44.647	40.433		1.00	50.95
	1062	CB	TRP	130	43.933		37.422	1.00	50.95
	1063	CG	TRP	130	43.933	39.172	37.899	1.00	147.57
20	1064	CD2	TRP			39.505	38.701	1.00	147.57
20	1065	CE2		130	42.410	39.002	39.993	1.00	147.57
	1066		TRP	130	41.230	39.650	40.406	1.00	147.57
		CE3	TRP	130	43.023	38.088	40.853	1.00	147.57
	1067	CD1	TRP	130	41.744	40.394	38.378	1.00	147.57
25	1068	NE1	TRP	130	40.841	40.486	39.400	1.00	147.57
25	1069	CZ2	TRP	130	40.636	39.388	41.632	1.00	147.57
	1070	CZ3	TRP	130	42.436	37.831	42.068	1.00	147.57
	1071	CH2	TRP	130	41.257	38.488	42.454	1.00	147.57
	1072	С	TRP	130	46.011	40.129	36.846	1.00	50.95
	1073	0	TRP	130	46.184	40.232	35.628	1.00	50.95
30	1074	N	TYR	131	46.980	39.759	37.670	1.00	143.97
	1075	CA	TYR	131	48.287	39.493	37.101	1.00	143.97
	1076	CB	TYR	131	49.320	39.136	38.170	1.00	125.03
	1077	CG	TYR	131	50.636	38.736	37.544	1.00	
	1078	CD1	TYR	131	51.129	39.426	36.443	1.00	125.03
35	1079	CE1	TYR	131	52.276	39.026	35.794	1.00	125.03
	1080	CD2	TYR	131	51.347	37.634			125.03
	1081	CE2	TYR	131	52.511		37.995	1.00	125.03
	1082	CZ	TYR	131	52.964	37.230	37.352	1.00	125.03
	1083	OH OH	TYR	131		37.927	36.249	1.00	125.03
40	1084	C	TYR		54.078	37.504	35.573	1.00	125.03
70	1085	ŏ		131	48.285	38.404	36.033	1.00	143.97
	1086	N	TYR	131	48.818	38.608	34.943	1.00	143.97
	1087		GLU	132	47.700	37.254	36.351	1.00	105.73
		CA	GLU	132	47.628	36.119	35.427	1.00	105.73
45	1088	CB	GLU	132	47.113	36. 56 0	34.053	1.00	172.31
43	1089	CG	GLU	132	46.992	35.425	33.034	1.00	172.31
	1090	CD	GLU	132	46.449	35.896	31.695	1.00	172.31
	1091	OE1	GLU	132	45.321	36.436	31.670	1.00	172.31
	1092	OE2	GLU	132	47.148	35.724	30.670	1.00	172.31
50	1093	С	GLU	132	48.962	35.397	35.256	1.00	105.73
50	1094	0	GLU	152	50.022	35.935	35.552	1.00	105.73
	1095	N	ASN	133	48.887	34.172	34.758	1.00	117.87
	1096	CA	ASN	133	50.061	33.336	34.554	1.00	117.87
	1097	CB	ASN	133	50.894	33.311	35.844	1.00	184.60
	1098	CG	ASN	133	52.234	32.621	35.675	1.00	184.60
55	1099	OD1	ASN	133	52.612	32.227	34.573	1.00	184.60
	1100	ND2	ASN	133	52.966	32.479	36.775	1.00	184.60
	1101	C	ASN	133	49.470	31.961	34.285		
	1102	ō	ASN	133	48.297	31.741	34.563	1.00	117.87
	1103	Ň	HIS	134 ·	50.248	31.038		1.00	117.87
60	1104	ĊA	HIS	134	49.714	29.700	33.732	1.00	156.61
••	1105	CB	HIS	134			33.509	1.00	156.61
	1106	CG	HIS		50.697	28.835	32.710	1.00	161.49
	1107	CD2		134	50.137	27.491	32.325	1.00	161.49
	1107		HIS	134	50.423	26.249	32.787	1.00	161.49
65		ND1	HIS	134	49.130	27.348	31.409	1.00	161.49
05	1109	CE1	HIS	134	48.802	26.061	31.313	1.00	161.49
	1110	NE2	HIS	134	49.569	25.382	32.136	1.00	161.49
	1111	C	HIS	134	49.547	29.124	34.915	1.00	156.61
	1112	0	HIS	134	49.172	27.967	35.093	1.00	156.61
70	1113	N	ASN	135	49.821	29.965	35.910	1.00	97.51
70	1114	CA	ASN	135	49.755	29.570	37.304	1.00	97.51

	1115	СВ	ASN	135	51.160	29.704	37.934	1.00	110.39
	1116	CG	ASN	135	52.230	28.875	37.217	1.00	110.39
	1117 1118	OD1 ND2	ASN ASN	135	51.990	27.742	36.801	1.00	110.39
5	1119	C	ASN	135 135	53.438 48.729	29.433 30.282	37.117	1.00	110.39
	1120	ŏ	ASN	135	48.097	29.646	38.193 39.031	1.00	97.51
	1121	Ň	ILE	136	48.542	31.589	38.037	1.00 1.00	97.51
	1122	CA	ILE	136	47.600	32.267	38.943	1.00	101.73 101.73
10	1123	CB	ILE	136	48.307	32.728	40.212	1.00	31.25
10	1124	CG2	ILE	136	47.296	33.031	41.311	1.00	31.25
	1125 1126	CG1	ILE	136	49.240	31.649	40.728	1.00	31.25
	1127	CD1 C	ILE	136	49.753	31.893	42.146	1.00	31.25
	1128	ŏ	ILE	136 136	46.867 46.274	33.476 33.477	38.424	1.00	101.73
15	1129	Ň	SER	137	46.901	34.498	37.354 39.257	1.00 1.00	101.73
	1130	CA	SER	137	46.286	35.780	39.011	1.00	57.41 57.41
	1131	CB	SER	137	44.901	35.617	38.380	1.00	67.48
	1132	OG	SER	137	44.052	35.011	39.328	1.00	67.48
20	1133	C	SER	137	46.183	36.488	40.392	1.00	57.41
20	1134 1135	0 N	SER	137	45.619	35.936	41.348	1.00	57.41
	1136	GA CA	ILE	138 138	46.730 46.751	37.708 38.515	40.476	1.00	65.35
	1137	CB	ILE	138	48.186	38.693	41.708 42.184	1.00	65.35
	1138	CG2	ILE	138	48.232	39.050	43.659	1.00 1.00	90.30 90.30
25	1139	CG1	ILE	138	48.941	37.407	41.930	1.00	90.30
	1140	CD1	ILE	138	50.416	3 7.583	41.970	1.00	90.30
	1141	C	ILE	138	46.148	39.928	41.561	1.00	65.35
	1142 1143	0 N	ILE	138	46.060	40.471	40.456	1.00	65.35
30	1144	CA	THR	139 139	45.745 45.164	40.515	42.683	1.00	86.56
	1145	CB	THR	139	43.649	41.843 41.817	42.672 42.377	1.00	86.56
	1146	OG1	THR	139	43.399	41.192	41.115	1.00 1.00	127.73 127.73
	1147	CG2	THR	139	43.093	43.253	42.386	1.00	127.73
35	1148	Č	THR	139	45.331	42.466	44.043	1.00	86.56
33	1149	0	THR	139	45.198	41.779	45.051	1.00	86.56
	1150 1151	N CA	ASN ASN	140 140	45.624	43.763	44.089	1.00	96.52
	1152	CB	ASN	140	45. 75 3 46.301	44.415 45.834	45.370	1.00	96.52
	1153	ČĠ	ASN	140	46.721	46.427	45.214 46.534	1.00 1.00	124.36
40	1154	OD1	ASN	140	46.321	45.925	47.576	1.00	124.36 124.36
	1155	ND2	ASN	140	47.512	47.492	46.515	1.00	124.36
	1156	C	ASN	140	44.325	44.432	45.916	1.00	96.52
	1157 1158	0 N	ASN	140	43.390	44.861	45.244	1.00	96.52
45	1159	ČA	ALA ALA	141 141	44.168	43.921	47.126	1.00	84.53
	1160	CB	ALA	141	42.876 43.022	43.846 43.170	47.769 49.104	1.00	84.53
	1161	Č	ALA	141	42.197	45.188	47.942	1.00 1.00	49.12 84.53
	1162	0	ALA	141	42.778	46.143	48.459	1.00	84.53
50	1163	N	THR	142	40.942	45.223	47.514	1.00	86.11
30	1164	CA	THR	142	40.094	46.401	47.593	1.00	86.11
	1165 1166	CB OG1	THR THR	142	39.660	46.860	46.184	1.00	85.26
	1167	CG2	THR	142 142	40.816 38.793	47.143 48.102	45.386 46.268	1.00	85.26
	1168	č	THR	142	38.847	45.955	46.208 48.337	1.00 1.00	85.26
55	1169	0	THR	142	38.577	44.766	48.411	1.00	86.11 86.11
	1170	N	VAL	143	38.089	46.889	48.897	1.00	1 u j.48
	1171	CA	VAL	143	36.863	46.494	49.566	1.00	105.48
	1172 1173	CB CC1	VAL	143	36.240	47.653	50.360	1.00	154.19
60	1174	CG1 CG2	VAL VAL	143 143	35.816	48.766	49.413	1.00	154.19
-	1175	C	VAL	143	35.055 35.917	47.144 46.092	51.159	1.00	154.19
	1176	ŏ	VAL	143	34.937	45.371	48. 428 48. 63 5	1.00 1.00	105.48 105.48
	1177	N	GLU	144	36.238	46.560	47.223	1.00	97.40
<i>C</i> =	1178	CA	GLU	144	35.454	46.269	46.022	1.00	97.40
65	1179	CB	GLU	144	35.815	47.241	44.905	1.00	151.67
	1180	CG	GLU	144	35.304	48.645	45.100	1.00	151.67
	1181 1182	CD OE1	GLU GLU	144	35.772	49.574	44.000	1.00	151.67
	1183	OE2	GLU	144 144	35.580 36.330	49.236 50.643	42.811	1.00	151.67
70	1184	Č	GLU	144	35.682	44.857	44.324 45.517	1.00 1.00	151.67
							70.017	1.00	97.40

	1185	0	GLU	144	34.784	44.232	44.963	1.00	97.40
	1186	N O4	ASP	145	36.905	44.376	45.690	1.00	99.27
	1187 1188	CA CB	ASP ASP	145	37.266	43.040	45.268	1.00	99.27
5	1189	CG	ASP	145 145	38.759 39.616	42.808 43.652	45.491	1.00	103.93
_	1190	OD1	ASP	145	39.333	43.649	44.576 43.359	1.00	103.93
	1191	OD2	ASP	145	40.568	44.306	45.064	1.00 1.00	103.93
	1192	C	ASP	145	36.461	42.016	46.042	1.00	103.93 99.27
• •	1193	0	ASP	145	36.442	40.847	45.687	1.00	99.27
10	1194	N	SER	146	35.793	42.455	47.104	1.00	71.52
	1195	CA	SER	146	34.985	41.545	47.900	1.00	71.52
	1196 1197	CB OG	SER	146	34.386	42.266	49.105	1.00	85.74
	1198	C	SER	146 146	35.371	42.424	50.111	1.00	85.74
15	1199	ŏ	SER	146	33.900 33.469	40.948 41.569	47.012 46.036	1.00	71.52
	1200	Ň	GLY	147	33.493	39.724	47.333	1.00 1.00	71.52 96.87
	1201	CA	GLY	147	32.481	39.051	46.546	1.00	96.87 96.87
	1202	С	GLY	147	32.739	37.567	46.394	1.00	96.87
20	1203	0	GLY	147	33.695	CT 032	46.955	1.00	96.87
20	1204	N.	THR	148	31.883	26.908	45.617	1.00	103.30
	1205	CA	THR	148	31.975	35.469	45.377	1.00	103.30
	1206 1207	CB OG1	THR	148	30.596	34.819	45.355	1.00	64.66
	1208	CG2	THR	148 148	30.231 29.559	34.568	43.990	1.00	64.66
25	1209	C	THR	148	32.629	35.746 35.167	45.982 44.035	1.00 1.00	64.66
	1210	Ō	THR	148	32.261	35.726	42.998	1.00	103.30 103.30
	1211	N	TYR	149	33.586	34.253	44.059	1.00	77.50
	1212	CA	TYR	149	34.294	33.888	42.853	1.00	77.50
30	1213	CB	TYR	149	35.798	34.053	43.059	1.00	78.57
30	1214	CG	TYR	149	36.237	35.491	43.209	1.00	78.57
	1215 1216	CD1 CE1	TYR	149	35.965	36.210	44.372	1.00	78.57
	1217	CD2	TYR TYR	149 149	36.349	37.540 36.444	44.492	1.00	78.57
	1218	CE2	TYR	149	36.907 37.291	36.141 37.463	42.169 42.277	1.00 1.00	78.57
35	1219	CZ	TYR	149	37.012	38.161	43.437	1.00	78.57. 78.57
	1220	OH	TYR	149	37.388	39.485	43.527	1.00	78.57
	1221	C	TYR	149	34.018	32.469	42.439	1.00	77.50
	1222	0	TYR	149	33.424	31.694	43.185	1.00	77.50
40	1223 1224	N CA	TYR	150	34.473	32.150	41.232	1.00	44.44
70	1225	CA CB	TYR TYR	150	34.335	30.823	40.648	1.00	44.44
	1226	CG	TYR	150 150	32.851 32.132	30.446 30.968	40.588	1.00	66.36
	1227	CD1	TYR	150	32.205	30.288	39.376 38.157	1.00 1.00	66.36 66.36
	1228	CE1	TYR	150	31.585	30.776	37.034	1.00	66.36
45	1229	CD2	TYR	150	31.411	32.156	39.433	1.00	66.36
	1230	CE2	TYR	150	30.788	32.655	38.315	1.00	66.36
	1231	CZ	TYR	150	30.878	31.959	37.120	1.00	66.36
	1232 1233	ОН	TYR	150	30.243	32.436	36.007	1.00	66.36
50	1234	C	TYR TYR	150	34.957	30.881	39.240	1.00	44.44
50	1235	Ň	CYS	150 151	34.796 35.677	31.872 29.842	38.536	1.00	44.44
	1236	ĊA	CYS	151	36.290	29.853	38.833 37.513	1.00 1.00	64.10
	1237	C	CYS	151	35.713	28.792	36.616	1.00	64.10 64.10
	1238	0	CYS	151	35.015	27.897	37.067	1.00	64.10
55	1239	CB	CYS	151	37.813	29.668	37.612	1.00	75.24
	1240	SG	273	151	38.407	28.123	38.380	1.00	75.24
	1241 1242	N	THR	152	36.021	28.904	35.334	1.00	63.66
	1243	CA CB	THR THR	152	35.553	27.971	34.330	1.00	63.66
60	1244	OG1	THR	152 152	34.453 35.025	28.599 29.615	33.459	1.00	48.15
	1245	CG2	THR	152	33.360	29.204	32.619 34.341	1.00 1.00	48.15
	1246	C	THR	152	36.779	27.708	33.479	1.00	48.15 63.66
	1247	0	THR	152	37.709	28.512	33.473	1.00	63.66
6 5	1248	N	GLY	153	36.786	26.586	32.770	1.00	68.75
65	1249	CA	GLY	153	37.917	26.256	31.929	1.00	68.75
	1250	C	GLY	153	37.588	24.988	31.180	1.00	68.75
	1251 1252	O N	GLY	153	36.783	24.186	31.649	1.00	68.75
	1252	ČA	LYS LYS	154 154	38.192 37.936	24.800	30.016	1.00	56.66
70	1254	CB	LYS	154	37.936 37.984	23.603 23.917	29.248 27. 7 51	1.00	56.66
						_0.017	27.731	1.00	131.33

	1255	CG	LYS	154	37.756	22.699	26.874	1.00	101.00
	1256	CD	LYS	154	38.014	22.985	25.401	1.00	131.33 131.33
	1257	CE	LYS	154	37.989	21.684	24.596	1.00	131.33
_	1258	NZ	LYS	154	38.322	21.823	23.146	1.00	131.33
5	1259	С	LYS	154	38.932	22.501	29.582	1.00	56.66
	1260	0	LYS	154	40.141	22.713	29.562	1.00	56.66
	1261	N	VAL	155	38.412	21.321	29.913	1.00	93.07
	1262	CA	VAL	155	39.260	20.162	30.203	1.00	93.07
10	1263	CB	VAL	155	38.924	19.490	31.544	1.00	78.48
10	1264	CG1	VAL	155	40.072	18.590	31.955	1.00	78.48
	1265 1266	CG2 C	VAL VAL	155 155	38.659	20.536	32.606	1.00	78.48
	1267	ŏ	VAL	155	38.956 37.802	19.179 19.005	29.095 28.719	1.00	93.07
	1268	Ň	TRP	156	39.992	18.547	28.566	1.00 1.00	93.07
15	1269	ČA	TRP	156	39.826	17.597	27.476	1.00	110.90 110.90
	1270	СВ	TRP	156	39.093	16.344	27.963	1.00	64.42
	1271	CG	TRP	156	39.889	15.530	28.952	1.00	64.42
	1272	CD2	TRP	156	41.144	14.909	28.711	1.00	64.42
•	1273	CE2	TRP	156	41.538	14.254	29.912	1.00	64.42
20	1274	CE3	TRP	156	41.989	14.836	27.593	1.00	64.42
	1275	CD1	TRP	156	39.562	15.241	30.265	1.00	64.42
	1276	NE1	TRP	156	40.550	14.478	30.845	1.00	64.42
	1277 1278	CZ2 CZ3	TRP TRP	156 156	42.732	13.535	30.029	1.00	64.42
25	1279	CH2	TRP	156	43.178 43.539	14.125 13.482	27.705 28.919	1.00	64.42
	1280	Č	TRP	156	39.063	18.269	26. 33 5	1.00 1.00	64.42 110.90
	1281	õ	TRP	156	39.674	18.848	25.432	1.00	110.90
	1282	N	GLN	157	37.738	18.225	26.366	1.00	82.18
	1283	CA	GLN	157	36.980	18.857	25.298	1.00	82.18
30	1284	CB	GLN	157	36.566	17.802	24.260	1.00	143.76
	1285	CG	GLN	157	37.656	16.778	23.860	1.00	143.76
	1286	CD	GLN	157	37.147	15.761	22.835	1.00	143.76
	1287 1288	OE1	GLN	157	35.954	15.470	22.790	1.00	
35	1289	NE2 C	GLN GLN	157 157	38.050	15.211	22.025	1.00	143.76
33	1290	ŏ	GLN	157	35.737 34.910	19.520 20.068	25.889 25.166	1.00	82,18
	1291	Ň	LEU	158	35.620	19.488	27.213	1.00 1.00	82.18 73.39
	1292	CA	LEU	158	34.443	20.030	27.881	1.00	73.39 73.39
	1293	CB	LEU	158	33.835	18.977	28.773	1.00	92.19
40	1294	CG	LEU	158	34.030	17.598	28.187	1.00	92.19
	1295	CD1	LEU	158	33.153	16.628	28.944	1.00	92.19
	1296	CD2	LEU	158	33.664	17.618	26.702	1.00	92.19
	1297 1298	C	LEU	158	34.658	21.254	28.724	1.00	73.39
45	1299	0 N	ASP	158 159	35.763	21.525	29.180	1.00	73.39
43	1300	CA	ASP	159	33.564 33.615	21.955 23.183	28.992 29.761	1.00	13.69
	1301	CB	ASP	159	32.773	24.249	29.074	1.00 1.00	43.69 96.10
	1302	CG	ASP	159	33.085	24.373	27.594	1.00	86.10
	1303	OD1	ASP	159	34,289	24.477	27.249	1.00	86.10
50	1304	OD2	ASP	159	32.128	24.374	26.778	1.00	86.10
	1305	C	ASP	159	33.103	23.041	31.167	1.00	43.69
	1306	0	ASP	159	31.900	22.907	31.357	1.00	43.69
	1307	N CA	TYR	160	33.976	23.093	32.170	1.00	43.37
55	1308 1309	CA CB	TYR TYR	160	33.462	22.999	33.539	1.00	43.37
33	1310	CG CG	TYR	160 160	34.282 34.323	22.024 20.649	34.398 33.808	1.00	105.78
	1311	CD1	TYR	160	35.087	20.415	32.671	1.00 1.00	105.78 105.78
	1312	CE1	TYR	160	35.035	19.211	32.001	1.00	105.78
	1313	CD2	TYR	160	33.500	19.617	34.286	1.00	105.78
60	1314	CE2	TYR	160	33.436	18.387	33.612	1.00	105.78
	1315	CZ	TYR	160	34.209	18.205	32.458	1.00	105.78
	1316	ОH	TYR	160	34.143	17.068	31.692	1.00	105.78
	1317	C	TYR	160	33.340	24.331	34.265	1.00	43.37
65	1318	O	TYR	160	33.620	25.407	33.736	1.00	43.37
05	1319 1320	N CA	GLU	161	32.893	24.230	35.498	1.00	53.88
	1321	CB	GLU	161 161	32.709 31.270	25.388 25.866	36.333	1.00	53.88
	1322	CG	GLU	161	30.834	25.866 26.756	36.228 37.346	1.00 1.00	72.58 72.58
	1323	CD	GLU	161	29.490	20.730 27.372	37.0 6 7	1.00	72.58 72.58
70	1324	OE1	GLU	161	28.930	28.016	37.992	1.00	72.58
									·

	1325 1326	OE2 C	GLU	161 161	29.002 33.002	27.212 24.902	35.918 37.725	1.00	72.58
	1327	ŏ	GLU	161	32.658	23.765	38.063	1.00 1.00	53.88
	1328	Ň	SER	162	33.651	25.737	38.523	1.00	53.88
5	1329	CA	SER	162	33.967	25.330	39.868	1.00	54.33 54.33
	1330	CB	SER	162	35.289	25.931	40.327	1.00	58.04
	1331	OG	SER	162	35.183	27.339	40.452	1.00	58.04
	1332	Ç	SER	162	32.868	25.781	40.794	1.00	54.33
10	1333	0	SER	162	31.975	26.508	40.391	1.00	54.33
10	1334	N	GLU	163	32.923	25.298	42.028	1.00	45.72
	1335 1336	CA	GLU	163	31.959	25.656	43.045	1.00	45.72
	1337	CB CG	GLU GLU	163	32.210	24.853	44.313	1.00	129.00
	1338	CD	GLU	163 163	31.766 30.264	23.437 23.378	44.264	1.00	129.00
15	1339	OE1	GLU	163	29.702	24.206	44.300 45.051	1.00	129.00
	1340	OE2	GLU	163	29.657	22.531	43.595	1.00 1.00	129.00
	1341	C	GLU	163	32.259	27.102	43.356	1.00	129.00 45.72
	1342	0	GLU	163	33.425	27.501	43.399	1.00	45.72
20	1343	N	PRO	164	31.219	27.914	43.576	1.00	67.32
20	1344	CD	PRO	164	29.759	27.742	43.567	1.00	86.92
	1345	CA	PRO	164	31.578	29.289	43.884	1.00	67.32
	1346 1347	CB CG	PRO	164	30.227	29.992	43.934	1.00	86.92
	1347	. C	PRO PRO	164 164	29.312	28.921	44.383	1.00	86.92
25	1349	ŏ	PRO	164	32.342 32.402	29.348	45.213	1.00	67.32
	1350	Ň	LEU	165	32.943	28.372 30.507	45.973 45.461	1.00	67.32
	1351	CA	LEU	165	33.699	30.751	46.675	1.00 1.00	65.83
	1352	СВ	LEU	165	35.183	30.549	46.392	1.00	65.83 49.81
	1353	CG	LEU	165	36.123	30.662	47.579	1.00	49.81
30	1354	CD1	LEU	165	35.645	29.788	48.747	1.00	49.81
	1355	CD2	LEU	165	37.495	30.247	47.100	1.00	49.81
	1356	C	LEU	165	33.424	32.177	47.156	1.00	65.83
	1357 1358	0	LEU	165	33.235	33.094	46.344	1.00	65.83
35	1358	N CA	ASN ASN	166 166	33.376	32.358	48.473	1.00	106.87
55	1360	CB	ASN	166	33.117 31.975	33.676 33.597	49.033	1.00	106.87
	1361	ČĠ	ASN	166	30.601	33.541	50.055 49.380	1.00	138.19
	1362	OD1	ASN	166	30.053	32.448	49.150	1.00 1.00	138.19 138.19
	1363	ND2	ASN	166	30.075	34.724	49.034	1.00	138.19
40	1364	С	ASN	166	34.356	34.348	49.629	1.00	106.87
	1365	0	ASN	166	34.960	33.853	50.578	1.00	106.87
	1366	N .	ILE	167	34.719	35.487	49.041	1.00	79.40
	1367 1368	CA	ILE	167	35.882	36.278	49.444	1.00	79.40
45	1369	CB CG2	ILE ILE	167 167	36.849	36.419	48.260	1.00	72.10
	1370	CG1	ILE	167	37.796 37.558	37.571 35.074	48.491	1.00	72.10
	1371	CD1	ILE	167	38.444	35.007	48.042 46.826	1.00 1.00	72.10
	1372	C	ILE	167	35.502	37.662	49.951	1.00	72.10 79.40
~~	1373	0	ILE	167	34.768	38.397	49.295	1.00	79.40 79.40
50	1374	N	THR	168	36.013	38.003	51.126	1.00	78.85
	1375	CA	THR	168	35.727	39.284	51.750	1.00	78.85
	1376	CB	THR	168	34.988	39.074	53.096	1.00	110.41
	1377 1378	CG2	THR	168	33.724	38.444	52.850	1.00	110.41
55	1379	C	THR THR	168	34.753	40.400	53.805	1.00	110.41
50	1380	ŏ	THR	168 168	37.012 37.999	40.064 39.523	52.000	1.00	78.85
	1381	Ň	VAL	169	36.997	41.338	52.508 51.634	1.00 1.00	78.85
	1382	CA	VAL	169	38.163	42.177	51.829	1.00	91.78 91.78
	1383	CB	VAL	169	38.475	42.968	50.576	1.00	74.43
60	1384	CG1	VAL	169	39.886	43.524	50.663	1.00	74.43
	1385	CG2	VAL	169	38.303	42.079	49.361	1.00	74.43
	1386	C	VAL	169	37.898	43.146	52. 96 5	1.00	91.78
	1387 1388	0	VAL	169	37.524	44.297	52.738	1.00	91.78
65	1389	N CA	ILE	170 170	38.085	42.676	54.192	1.00	138.54
55	1390	CB	ILE	170 170	37.838 38.201	43.522	55.342	1.00	138.54
	1391	CG2	ILE	170	38.201	42.815 43.798	56.649 57.810	1.00	99.90
	1392	CG1	ILE	170	37.253	41.628	57.810 56.869	1.00 1.00	99.90
70	.1393	CD1	ILE	170	37.436	40.914	58.193	1.00	99.90 99.90
70	1394	С	ILE	170	38.598	44.837	55.255	1.00	138.54
								-	· - ·

	1395 1396	O N	ILE LYS	170 171	39.816 37.856	44.880 45.912	55.419 55.002	1.00 1.00	138.54 166.26
	1397	CA :	LYS	171	38.420	47.254	54.878	1.00	166.26
_	1398	CB ·	LYS	171	37.322	48.228	54.430	1.00	153.43
5	1399	cg	LYS	171	37.806	49.608	53.987	1.00	153.43
	1400 1401	CD	LYS	171	36.637	50.449	53.489	1.00	153.43
	1401	CE NZ	LYS LYS	171	37.084	51.765	52.885	1.00	153.43
	1403	C	LYS	171 171	35.907	52.541	52.405	1.00	153.43
10	1404	ŏ	LYS	171	39.042 39.710	47.737 46.977	56.189	1.00	166.26
	1405	C1	NAG	221	52.176	13.407	56.894	1.00	166.26
	1406	C2	NAG	221	52.353	13.121	48.424 46.936	1.00	124.69
	1407	N2	NAG	221	51.119	13.440	46.226	1.00 1.00	124.69
	1408	C7	NAG	221	51.096	14.392	45.292	1.00	124.69
15	1409	07	NAG	221	52,111	14.981	44.911	1.00	124.69 124.69
	1410	C8	NAG	221	49.744	14.746	44.682	1.00	124.69
	1411	C3	NAG	221	52.712	11.631	46.753	1.00	124.69
	1412	03	NAG	221	53.109	11.400	45.409	1.00	124.69
20	1413	C4	NAG	221	53.847	11.168	47.703	1.00	124.69
20	1414	04	NAG	221	53.876	9.724	47.741	1.00	124.69
	1415	C5	NAG	221	53.635	11.683	49.139	1.00	124.69
	1416	O5	NAG	221	53.371	13.099	49.133	1.00	124.69
	1417 1418	C6 O6	NAG	221	54.853	11.458	50.023	1.00	124.69
25	1419	C1	NAG NAG	221 222	54.616	11.876	51.361	1.00	124.69
23	1420	C2	NAG	222	55.008	9.074	47.260	1.00	186.41
	1421	N2	NAG	222	55.394 55.812	7.926	48.219	1.00	186.41
	1422	C7	NAG	222	55.243	8.470 8.053	49.500 50.628	1.00	186.41
	1423	07	NAG	222	54.288	7.270	50.654	1.00 1.00	186.41
30	1424	C8	NAG	222	55.823	8.589	51.930	1.00	186.41 186.41
	1425	СЗ	NAG	222	56.531	7.079	47.623	1.00	186.41
	1426	O3	NAG	222	56.764	5.942	48.445	1.00	186.41
	1427	C4	NAG	222	56.174	6.622	46.205	1.00	186.41
25	1428	04	NAG	222	57.286	5.958	45.616	1.00	186.41
35	1429	C5	NAG	222	55.775	7.830	45. 34 5	1.00	186.41
	1430	O5	NAG	222	54.681	8.548	45.9 63	1.00	186.41
	1431 1432	C6 O6	NAG	222	55.302	7.412	43.963	1.00	186.41
	1433	C1	NAG NAG	222 242	54.550	8.444	43.340	1.00	186.41
40	1434	C2	NAG	242 242	36.605 36.383	17.603 16.211	61.014	1.00	57.79
	1435	N2	NAG	242	37.564	15.387	60.400 60.550	1.00	57.79
	1436	C7	NAG	242	37.706	14.678	61.665	1.00 1.00	57.79 57.70
	1437	07	NAG	242	36.949	14.833	62.624	1.00	57.79 57.79
	1438	C8	NAG	242	38.838	13.642	61.747	1.00	57.79
45	1439	C3	NAG	242	36.035	16.395	58.924	1.00	57.79
	1440	O3	NAG	242	35.897	15.142	58.256	1.00	57.79
	1441	C4	NAG	242	34.754	17.226	58.828	1.00	57.79
	1442	04	NAG	242	34.498	17.491	57.446	1.00	57.79
50	1443	C5	NAG	242	34.988	18.570	59.547	1.00	57.79
50	1444 1445	05 C6	NAG	242	35.393	18.365	60.921	1.00	57.79
	1446	06	NAG NAG	242	33.781	19.492	59.556	1.00	57.79
	1447	C1		242	34.170	20.863	59.403	1.00	57.79
	1448	C2	NAG NAG	243 243	33.499 33 <i>.2</i> 79	16.811 17.515	56.792 55.463	1.00	110.47
55	1449	N2	NAG	243	32.859	18.887	55.463 55.667	1.00	110.47
	1450	C7	NAG	243	33.584	19.876	55.149	1.00 1.00	110.47
	1451	07	NAG	243	34.659	19.682	54.574	1.00	110.47 110.47
	1452	C8	NAG	243	33.036	21.294	55.277	1.00	110.47
<u></u>	1453	C3	NAG	243	32.273	16.758	54.610	1.00	110.47
60	1454	03	NAG	243	32.168	17.391	53.345	1.00	110.47
	1455	C4	NAG	243	32.746	15.314	54.413	1.00	110.47
	1456	O4	NAG	243	31.718	14.574	5 3.705	1.00	110.47
	1457	C5	NAG	243	33.038	14.665	55.789	1.00	110.47
65	1458 1459	`O5	NAG	243	33.967	15.474	56.555	1.00	110.47
UJ.	1459	C6 O6	NAG	243	33.671	13.290	55.655	1.00	110.47
	1461	C1	nag. Man	243	34.005	12.749	56.924	1.00	110.47
	1462	C2	MAN	244 244	32.107	13.609	52.777 52.000	1.00	99.82
	1463	02	MAN	244	31.311 29.925	12.313 12.615	53.039 53.134	1.00	99.82
70	1464	ČŠ	MAN	244	31.545	11.278	53.134 51.921	1.00	99.82
-		· -		3		11.270	31.321	1.00	99.82

	1465 1466	03 C4	MAN MAN	244 244	30.713 31.266	10.135 11.903	52.110 50.555	1.00 1.00	99.82 99.82
	1467 1468	O4 .	MAN	244	31.547	10.959	49.527	1.00	99.82
5	1469	C5 O5	MAN MAN	244 244	32.168	13.132	50.412	1.00	99.82
_	1470	C6	MAN	244	31.840 32.132	14.107 13.816	51.442	1.00	99.82
	1471	06	MAN	244	30.954	14.583	49.038 48.837	1.00	99.82
	1472	C1	NAG	250	57.134	13.804	64.271	1.00 1.00	99.82
	1473	C2	NAG	250	57.130	13.286	65.723	1.00	196.94 196.94
10	1474	N2	NAG	250	58.492	13.078	66.175	1.00	196.94
	1475	C7	NAG	250	58. 87 1	13.481	67.385	1.00	196.94
	1476 1477	O7 C8	NAG NAG	250	58.184	14.217	68.096	1.00	196.94
	1478	C3	NAG	250 250	60.225 56.359	12.994	67.883	1.00	196.94
15	1479	O3	NAG	250	56.224	11.960 11.547	65.803 67.156	1.00	196.94
	1480	C4	NAG	250	54.974	12.098	65.176	1.00 1.00	196.94 196.94
	1481	04	NAG	250	54.343	10.826	65.136	1.00	196.94
	1482	C5	NAG	250	55.102	12.658	63.758	1.00	196.94
20	1483 1484	O5 C6	NAG	250	55.794	13.927	63.783	1.00	196.94
20	1485	O6	NAG NAG	250 250	53.754 53.895	12.893	63.115	1.00	196.94
	1486	C1	NAG	250 274	45.966	13.367 34.168	61.783	1.00	196.94
	1487	C2	NAG	274	44.449	34.481	75.904 75.778	1.00	202.51
	1488	N2	NAG	274	44.020	34.633	74.386	1.00 1.00	202.51 202.51
25	1489	C7	NAG	274	42.782	34.284	74.009	1.00	202.51
	1490	07	NAG	274	42.000	33.685	74.755	1.00	202.51
	1491 1492	C8	NAG	274	42.322	34.648	72.599	1.00	202.51
	1492	C3 O3	NAG NAG	274	44.167	35.773	76.602	1.00	202.51
30	1494	C4	NAG	274 274	42.768 44.757	35.996 35.723	76.692	1.00	202.51
	1495	04	NAG	274	44.775	37.037	78.040 78.589	1.00 1.00	202.51
	1496	C5	NAG	274	46.191	35.157	78.058	1.00	202.51 202.51
	1497	Q5	NAG	274	46.265	33.950	77.282	1.00	202.51
35	1498 1499	C6	NAG	274	46.690	34.798	79.448	1.00	202.51
22	1500	O6 C1	nag Nag	274	47.729	33.828	79.381	1.00	202.51
	1501	C2	NAG	340 340	47.734 49.212	48.240 48.677	47.742	1.00	87.46
	1502	N2	NAG	340	50.123	47.546	47.819 47.707	1.00 1.00	87.46
40	1503	C7	NAG	340	50.634	47.210	46.522	1.00	87.46 87.46
40	1504	07	NAG	340	50.025	47.375	45.468	1.00	87.46
	1505	C8	NAG	340	52.024	46.596	46.490	1.00	87.46
	1506 1507	C3 O3	NAG NAG	340 340	49.416	49.457	49.129	1.00	87.46
	1508	C4	NAG	340 340	50.779 48.512	49.830 50.694	49.261	1.00	87.46
45	1509	04	NAG	340	48.730	51.749	49.007 49.989	1.00 1.00	87.46
	1510	C5	NAG	340	47.044	50.277	48.965	1.00	87.46 87.46
	1511	O5	NAG	340	46.834	49.391	47.812	1.00	87.46
	1512 1513	C6 O6	NAG	340	46.182	51.556	48.793	1.00	87.46
50	1514	C1	NAG NAG	340 341	44.848	51.307	48.368	1.00	87.46
50	1515	C2	NAG	341	49.306 50.167	51.566 52.801	51.238 51.506	1.00	143.93
	1516	N2	NAG	341	51.241	52.873	51. 50 6 50. 54 0	1.00 1.00	143.93 143.93
	1517	C7	NAG	341	51.195	53.774	49.564	1.00	143.93
55	1518	07	NAG	341	50.313	54.630	49.471	1.00	143.93
23	1519	C8	NAG	341	52.303	53.716	48.535	1.00	143.93
	1520 1521	C3 O3	NAG NAG	341	50.722	52.777	52.923	1.00	143.93
	1522	64	NAG	341 341	51.522 49.548	53.931 52.753	53.148	1.00	143.93
	1523	04	NAG	341	50.031	52.753 52.717	53.891 55.229	1.00	143.93
60	1524	C5	NAG	341	48.686	51.510	53.587	1.00 1.00	143.93 143.93
	1525	O5	NAG	341	48.239	51.510	52.203	1.00	143.93
	1526	C6	NAG	341	47.428	51.437	54.427	1.00	143.93
	1527 1528	O6 C1	NAG	341	46.455	50.627	53.780	1.00	143.93
65	1529	C2	NAG NAG	366 366	28.633	34.916	48.881	1.00	149.17
	1530	N2	NAG	366	27.879 28.118	34.326 32.897	50.081 50.186	1.00	149.17
	1531	C7	NAG	366	28.345	32.346	50.186 51.378	1.00 1.00	149.17
	1532	07	NAG	366	28.482	33.013	52.407	1.00	149.17 149.17
70	1533	C8	NAG	366	28.441	30.828	51.448	1.00	149.17
70	1534	C3	. NAG	36 6	26.372	34.552	49.949	1.00	149.17

	1535	03	NAG	366	25.761	34.256	51.198	1.00	140 17
	1536	C4	NAG	366	25,976	35.987	49.514	1.00	149.17
	1537	04	NAG	366	24.660	35.921	48.921	1.00	149.17
	1538	C5	NAG	366	26.928	36.592	48.459		149.17
5	1539	O 5	NAG	366	28.320	36.323	48.766	1.00	149.17
	1540	C6	NAG	366	26.769	38.111	48.368	1.00	149.17
	1541	O6	NAG	366	27.829	38.807	49.016	1.00	149.17
	1542	C1	NAG	367	23.729	36.910	49.196	1.00	149.17
	1543	C2	NAG	367	22.797	37.075		1.00	173.80
10	1544	N2	NAG	367	23.536	37.637	47.975	1.00	173.80
	1545	C7	NAG	367	23.834		46.860	1.00	173.80
	1546	07	NAG	367		36.896	45.796	1.00	173.80
	1547	C8	NAG		23.531	35.706	45.691	1.00	173.80
	1548	C3	NAG	367	24.586	37.593	44.674	1.00	173.80
15	1549	∝ ⊙3		367	21.617	37.991	48.311	1.00	173.80
1	1550	C4	NAG	367	20.711	38.025	47.218	1.00	173.80
			NAG	367	20.897	37.499	49.566	1.00	173.80
	1551	O4	NAG	367	19.890	38.438	49.924	1.00	173.80
	1552	C5	NAG	367	21.917	37.360	50. 705	1.00	173.80
20	1553	O5	NAG	367	22.977	36.460	50. 326	1.00	173.80
20	1554	C6	NAG	367	21.347	36.810	51. 995	1.00	173.80
	1555	O6	NAG	367	22.385	36.606	52.948	1.00	173.80

Table 9. PhFc ϵ RI α_{1-172} , Form T1, residue exposure

>>> coordinate set= pent63_8c1.pdb

	segid	resid	resname	access	access-main	access-side
	CCCC	4	LYS	22.3151	10.9559	31.4026
5	CCCC	5	PRO	1.1153	1.4307	0.6949
	CCCC	6	LYS	16.7221	1.1596	29.1721
	CCCC	7	VAL	1.5573	2.7252	0.0000
	CCCC	8	SER	8.9731	1.8795	23.1603
	CCCC	9	LEU	3.7370	4.7824	2.6917
10	CCCC	10	ASN	12.6673	0.9406	24.3940
	0000	11	PRO	8.2815	0.5829	18.5464
	CCCC	12	PRO	9.7742	2.0935	20.0152
	CCCC	13	TRP	1.5926	0.1230	2.1805
	CCCC	14	ASN	3.3766	0.2934	6.4597
15	CČCC	15	ARG	1.6352	0.0000	2.5696
	CCCC	16	ILE	1.1737	0.0003	2.3470
	CCCC	17	PHE	0.2696	0.0000	0.4237
	CCCC	18	LYS	8.1283	3.2126	12.0608
	CCCC	19	GLY	5.5800	5.5800	0.0000
20	CCCC	20	GĽÚ	3.3428	0.0000	6.0170
	CCCC	21	ASN	5.3342	3.9503	6.71 82
	CCCC	22	VAL	0.3267	0.4564	0.71 62 0.15 38
	CCCC	23	THR	5.3278	0.4364	
	CCCC	24	LEU	0.2562	0.0002	12.4107
25	CCCC	25	THR	4.7853	0.0002	0.5121 11.1657
	CCCC	26	CYS	0.2343	0.3249	
	CCCC	27	ASN	7.7637		0.0530
	CCCC	28	GLY		1.8546	13.6728
	CCCC	29	ASN	7.9103	7.9103	0.0000
30	CCCC	30	ASN	16.6538	7.7758	25.5318
50	CCCC	31		14.2106	9.9392	18.4821
	CCCC	32	PHE PHE	18.4293	8.6833	23.9984
	CCCC	33	GLU	6.9543 17.3275	6.9847	6.9370
	CCCC	34			4.6057	27.5049
35	CCCC	35	VAL	9.7070	3.0781	18.5455
33	CCCC	36	SER	14.3512	2.1631	38.7274
	CCCC	36 37	SER	7.0113	1.9003	17.2334
	CCCC		THR	0.7139	1.2493	0.0000
		38	LYS	8.3149	0.3194	14.7113
40	CCCC	39	TRP	0.0064	0.0013	0.0084
40	CCCC	40	THE	3.0089	0.0000	4.7283
	CCCC	41	HIS	3.3635	0.3462	5.3750
		42	ASN	5.9924	6.1741	5.8107
	CCCC	43	GLY	8.7956	8.7956	0.0000
45	CCCC	44	SER	10.0868	2.4356	25.3890
40	CCCC	45	LEU	14.4496	6.7421	22.1571
	CCCC	46	SER	4.8664	3.2655	8.0682
	CCCC	47	GLU	13.8158	4.4486	21.3095
	CCCC	48	GLU	3.7957	0.7742	6.2129
50	CCCC	49	THR	11.0308	0.0826	25.6285
50	CCCC	50	ASN	3.7680	0.9608	6.5753
	CCCC	51	SER	0.9943	0.0001	2.9826

	2222 2222	52 53 54	SER LEU ASN	2.8849 2.6956 7.0487	0.0003 0.0208 3.7820	8.6541 5.3704 10.3153
	CCCC	55	ILE	2.0484	1.5241	2.5727
5	CCCC	56	VAL	8.3718	1.8780	17.0302
	CCCC	57	ASN	6.8809	0.9872	12.7747
	CCCC	58	ALA	0.3689	0.4454	0.0628
	CCCC	59	LYS	8.8541	0.0311	15.9126
	CCCC	60	PHE	3.1986	0.2109	4.9058
10	CCCC	61	GLU	8.5928	0.1580	15.3407
	CCCC	62	ASP	4.2001	0.0802	8.3200
	CCCC	63	SER	0.1586	0.0000	0.4759
	CCCC	64	GLY	0.0205	0.0205	0.0000
	CCCC	65	GLU	3.1362	0.1046	5.5614
15	CCCC	66	TYR	0.7765	0.0000	1.1648
	CCCC	67	LYS	3.3029	0.0005	5.9449
	CCCC	68	CYS	0.0000	0.0000	0.0000
	CCCC	69	GLN	3.8782	0.0000	6.9808
	CCCC	70	HIS	2.2973	0.2891	3.6361
20	CCCC	71	GLN	15 .5567	6.4047	22.8783
	CCCC	72	GLN	18.9536	6.5187	28.9015
	CCCC	73	VAL	6.3773	2.6597	11.3340
•	CCCC	74	ASN	7.2490	0.8511	13.6469
	CCCC	75	GLU	9.5776	4.4490	13.6806
25	CCCC	76	SER	0.7222	1.0831.	0.0006
	CCCC	77	GLU	13.3681	1.0686	23.2077
	CCCC	78	PRO	2.7891	1.9776	3.8710
	CCCC	79	VAL	5.1775	0.7766	11.0455
	CCCC	80	TYR	3.7512	1.4544	4.8996
30	CCCC	81	LEU	0.2610	0.0000	0.5221
	CCCC	82	GLU	5.7107	0.0011	10.2784
	CCCC	83	VAL	1.5280	2.6739	0.0000
	CCCC	84	PHE	2.6808	0.7184	3.8022
	CCCC	85	SER	5.8787	5.8008	6.0345
35	CECC	86	ASP	6.0903	2.6973	9.4832
	CCCC	87	TRP	3.0930	0.2603	4.2261
	CCCC	88	LEU	0.0403	0.0675	0.0131
	CCCC	89	LEU	0.1021	0.0000	0.2041
	CCCC	90	LEU	0.0000	0.0000	0.0000
40	CCCC	91	GLN	0.2597	0.0000	0.4674
	CCCC	92	ALA	0.0596	0.0563	0.0730
	CCCC	93	SER	4.6788	3.0077	8.0211
	CCCC	94	ALA	8.5911	1.3052	37.7350
	CCCC	95	GLU	4.4767	1.5831	6.7916
45	CCCC	96	VAL	4.3906	4.6557	4.0371
	CCCC	97	VAL	1.4394	1.1406	1.8378
	CCCC	98	MET	13.6889	0.2044	27.1734
	CCCC	99	GLU	7.4 7 97	4.8677	9.5692
	CCCC	100	GLY	5.3567	5.3567	0.0000
50	CCCC	101	GLN	9.7722	0.0006	17.5894
	CCCC	102	PRO	9.4569	1.5764	19.9642
	CCCC	103	LEU	0.0179	0.0357	0.0000
	CCCC	104	PHE	6.2358	0.0000	9.7991
	CCCC	105	LEU	0.0474	0.0488	0.0461
55	CCCC	106	ARG	2.3314	0.0000	3.6636
	CCCC	107	CYS	0.7781	1.1549	0.0246

	CCCC	108	HIS	1.2171	0.3012	1.8277
	CCCC	109	GLY	1.2651	1.2651	0.0000
	CCCC	110	TRP	1.9508	0.3094	2.6074
	CCCC	111	ARG	7.1821	6.7612	7.4226
_		112	ASN	12.7243	3.8235	21.6251
5	CCCC	113	TRP	2.9331	3.2961	2.7878
	CCCC		ASP	11.7314	2.0501	21.4128
	CCCC	114		0.8918	0.6165	1.2589
	cccc	115	VAL	5.7191	0.0000	8.5787
	CCCC	116	TYR	10.9908	0.9471	19.0258
10	CCCC	117	LYS	0.0001	0.0000	0.0002
	CCCC	118	VAL		0.0007	9.4248
	CCCC	119	ILE	4.7127	0.0000	0.0091
	CCCC	120	TYR	0.0060	0.0150	5.4562
	CCCC	121	TYR	3.6424	0.8428	6.4150
15	CCCC	122	LYS	3.9385	7.2355	14.8840
	CCCC	123	ASP	11.0597	13.5829	0.0000
	CCCC	124	GLY	13.5829	0.5211	23.2611
	CCCC	125	GLU	13.1544		53.4477
	CCCC	126	ALA	15.0490	5.4493	12.7176
20	CCCC	127	LEU	9.4150	6.1124	19.4295
	CCCC	128	LYS	11.5717	1.7494	
	CCCC	129	TYR	10.5011	5.5905	12.9565
	CCCC	130	TRP	8.0873	0.9625	10.9373
	CCCC	131	TYR	11.7870	1.0734	17.1438
25	CCCC	132	GLU	12.6705	2.2279.	21.0247
	CCCC	133	ASN	5.3027	5.3599	5.2454
	CCCC	134	HIS	8.2476	1.2608	12.9055
	CCCC	135	ASN	1.2965	0.3213	2.2717
	CCCC	136	ILE	2.0165	1.3778	2.6552
30	CCCC	137	SER	9.9968	7.2656	15.4593
50	CCCC	138	ILE	3.6077	0.9873	6.2280
	CCCC	139	THR	15.8360	2.4317	33.7085
	CCCC	140	ASN	6.0823	3.6720	8.4926
	CCCC	141	ALA	0.0000	0.0000	0.0000
35	CCCC	142	THR	6.7820	0.1381	15.6405
<i>JJ</i>	CCCC	143	VAL	5.0630	1.4175	9.9237
	CCCC	144	GLU	14.1160	4.3532	21.9263
	CCCC	145	ASP	4.3317	0.0259	8.6374
	CCCC	146	SER	5.1283	3.0010	9.3829
40	CCCC	147	GLY	3.4210	3.4210	0.0000
70	CCCC	148	THR	5.2803	0.0914	12.1988
	CCCC	149	TYR	0.2014	0.0000	0.3021
	CCCC	150	TYR	3.7574	0.0000	5.6362
	CCCC	151	CYS	0.0001	0.0001	0.0000
45	CCCC	152	THR	3.8919	0.0107	9.0668
43	CCCC	153	GLY	1.0188	1.0188	0.0000
	CCCC	154	LYS	6.4238	0.0528	11.5207
	CCCC	155	VAL	0.4180	0.0000	0.9754
	CCCC	156	TRP	3.3279	3.7718	3.1504
50	CCCC	157	GLN	13.1268	3.2479	21.0299
50	CCCC	158	LEU	8.7018	0.1257	17.2778
	CCCC	159	ASP	14.2676	4.9595	23.5758
		160	TYR	2.2687	2.5573	2.1243
	0000	161	GLU	12.1767	4.4230	18.3798
	CCCC		SER	1.1841	1.7762	0.0000
55	CCCC	162		9.4913	0.1747	16.9445
	CCCC	163	GLU	J.43 13	J. 17 47	

				•		
	CCCC	164	PRO	9.7765	1.5124	20.7953
	CCCC	165	LEU	1.6495	0.1289	3.1701
	CCCC	166	ASN	3.4007	0.7824	6.0190
	CCCC	167	ILE	0.5293	1.0585	0.0000
_	CCCC	168	THR	3.2321	0.0380	7.4909
5	CCCC	169	VAL	0.0723	0.1266	0.0000
		170	ILE	2.2951	0.0689	4.5213
	CCCC	171	LYS	14.3432	12.9256	15.4773
	CCCC	221	NAG	11.7001	0.0000	11.7001
10	CCCC	222	NAG	14.4010	0.0000	14.4010
10	CCCC		NAG	7.1046	0.0000	7.1046
	CCCC	242		8.0078	0.0000	8.0078
	CCCC	243	NAG	16.5438	0.0000	16.5438
	CCCC	244	MAN		0.0000	16.2147
	CCCC	250	NAG	16.2147	0.0000	21.7742
15	CCCC	274	NAG	21.7742	0.0000	15.0979
	CCCC	335	NAG	15.0979	0.0000	17.6065
	CCCC	340	NAG	17.6065	0.0000	11.8776
	CCCC	366	NAG	11.8776	0.0000	19.0810
	CCCC	367	NAG	19.0810		23.3099
20	AAAA	4	LYS	15.9363	6.7194	
	AAAA	5	PRO	1.1488	1.4481	0.7498
	AAAA	6	LYS	13.8574	1.1896	23.9916
	AAAA	7	VAL	1.5646	2.7375	0.0007
	AAAA	8	SER	9.0558	1.9390	23.2893
25	AAAA	9	LEU	3.8393	4.9388	2.7398
	AAAA	10	ASN	12.5152	0.9543	24.0762
	AAAA	11	PRO	8.3710	0.5349	18.8192
	AAAA	12	PRO	9.8889	2.0781	20.3033
	AAAA	13	TRP	1.5673	0.1143	2.1485
30	AAAA	14	ASN	3.1275	0.2808	5.9741
	AAAA	15	ARG	1.6130	0.0057	2.5315
	AAAA	16	ILE	1.1993	0.0000	2.3986
	AAAA	17	PHE	0.2501	0.0000	0.3929
	AAAA	18	LYS	10.8021	3.4649	16.6720
35	AAAA	19	GLY	5. 693 9	5.6939	0.0000
	AAAA	20	GLU	3.4960	0.0003	6.2926
	AAAA	21	ASN	5.3970	4.0391	6.7548
	AAAA	22	VAL	0.2660	0.3430	0.1633
	AAAA	23	THR	5.2134	0.0418	12.1090
40	AAAA	24	LEU	0.2554	0.0007	0.5101
, -	AAAA	25	THR	4.8 6 55	0.0005	11.3521
	AAAA	26	CYS	0.2307	0.3194	0.0532
	AAAA	27	ASN	0.4259	0.2949	0.5569
	AAAA	28	GLY	4.4162	4.4162	0.0000
45	AAAA	29	ASN	7.6150	7.1438	8.0862
	AAAA	30	ASN	11.3939	10.0050	12.782 9
	AAAA	31	PHE	14.7556	4.8219	20.4320
	AAAA	32	PHE	2.7147	4.5718	1.6536
	AAAA	33	GLU	7.5248	4.4574	9.9787
50	AAAA	34	VAL	4.0858	3.0519	5.4642
50	AAAA	35	SER	14.4683	2.1629	39.0790
	AAAA	36	SER	6.9471	1.9207	16.9999
	AAAA	37	THR	0.7130	1.2478	0.0000
	AAAA	38	LYS	8.2623	0.2915	14.6390
55	AAAA	39	TRP	0.0071	0.0080	0.0067
JJ	AAAA	40	PHE	2.9948	0.0014	4.7054
	~~~~	70				

	AAAA	41	HIS	3.3204	0.4762	5.2166
	AAAA	42	ASN	6.4516	7.1677	5.7356
•	AAAA	43	GLY	9.6929	9.6929	0.0000
	AAAA	44	SER	12.5467	3.0596	31.5 <b>209</b>
5	AAAA	45	LEU	14.0527	6.3669	21.7524
J	AAAA	46	SER	5.9554	3.7890	10.2883
	AAAA	47	GLU	19.8848	8.0231	29.3741
	AAAA	48	GLU	6.1436	2.1551	9.3344
		<del>40</del> 49	THR	10.8974	0.0037	25.4223
10	AAAA	<del>49</del> 50	ASN	3.7283	0.9830	6.4736
10	AAAA		SER	1.0424	0.0007	3.1257
	AAAA	51	SER	2.9027	0.0000	8.7080
	AAAA	52		2.6315	0.0203	5.2426
	AAAA	53	LEU	7.1111	3.9443	10.2778
	AAAA	54	ASN	2.099ú	1.5522	2.6464
15	AAAA	55	ILE		1.8784	24.1489
	AAAA	56	VAL	11.4229	0.9862	17.5682
	AAAA	57	ASN	9.2772	0.3981	0.0062
	AAAA	58	ALA	0.3197	0.0175	24.3155
	AAAA	59	LYS	13.5164		5.5088
20	AAAA	60	PHE	3.5563	0.1394	15.2857
	AAAA	61	GLU	8.5716	0.1791	
	AAAA	62	ASP	4.2001	0.0591	8.3412
	AAAA	63	SER	0.1501	0.0000	0.4504
	AAAA	64	GLY	0.0335	0.0335	0.0000
25	AAAA	65	GLU	8.1768	0.0971 .	14.6406
	AAAA	66	TYR	0.7839	0.0002	1.1758
	AAAA	67	LYS	3.2196	0.0004	5.7951
	AAAA	68	CYS	0.0000	0.0000	0.0000
	AAAA	69	GLN	3.8577	0.0000	6.9439
30	AAAA	70	HIS	0.2845	0.2473	0.3093
	AAAA	71	GLN	14.8691	6.1965	21.8072
	AAAA	72	GLN	18.3340	6.2079	28.0348
	AAAA	73	VAL	3.2302	2.5357	4.1564
	AAAA	74	ASN	7.3440	0.8492	13.8389
35	AAAA	75	GLU	9.5554	4.4097	13.6718
	AAAA	76	SER	0.5321	0.7981	0.0000
	AAAA	77	GLU	16.0334	0.9282	28.1176
	AAAA	78	PRO	8.2987	5.2204	12.4031
	AAAA	79	VAL	5.9326	1.3229	12.0789
40	AAAA	80	TYR	6.7460	1.9053	9.1664
	AAAA	81	LEU	0.2734	0.0000	0.5469
	AAAA	82	GLU	5.7587	0.0007	10.3651
	AAAA	83	VAL	1.5339	2.6843	0.0000
	AAAA	84	PHE	2.7544	0.6865	3.9361
45	AAAA	85	SER	11.1143	5.9578	21.4274
	AAAA	86	ASP	6.1024	2.2574	9.9474
	AAAA	87	TRP	9.2004	0.2983	12.7613
	AAAA	88	LEU	0.0297	0.0543	0.0051
	AAAA	89	LEU	0.0927	0.0000	0.1854
50	AAAA	90	LEU	0.0001	0.0000	0.0002
<b>5</b> 0	AAAA	91	GLN	0.2535	0.0000	0.4563
	AAAA	92	ALA	0.0453	0.0480	0.0344
	AAAA	93	SER	4.6084	2.9327	7.9597
	AAAA	94	ALA	8.7098	1.2990	38.3529
<b>5</b> 5	AAAA	95	GLU	7.3017	1.5643	11.8916
<i>33</i>	AAAA	96	VAL	12.9692	4.7889	23.8762
			•	· ·		

	AAAA	97	VAL .	1.4036	1.0908	1.8207
	AAAA	98	MET	7.3760	0.2425	14.5094
•	AAAA	99	GLU	7.1208	4.6443	9.1019
	AAAA	100	GLY	5.2380	5.2380	0.0000
5	AAAA	101	GLN	3.2910	0.0195	5.9082
5	AAAA	102	PRO	5.1174	1.6052	9.8002
	AAAA	103	LEU	0.0323	0.0600	0.0045
	AAAA	104	PHE	6.3337	0.0009	9.9525
	AAAA	105	LEU	0.0742	0.0597	0.0887
10	AAAA	106	ARG	2.3217	0.0000	3.6484
10	AAAA	107	CYS	0.7916	1.1873	0.0000
	AAAA	108	HIS	1.2205	0.3014	1.8333
	AAAA	109	GLY	1.3688	1.3688	0.0000
	AAAA	110	TRP	4.3961	0.3129	6.0293
15	AAAA	111	ARG	14.1659	6.8259	18.3603
13	AAAA	112	ASN	12.3349	3.8047	20.8651
	AAAA	113	TRP	7.3124	3.4188	8.8699
	AAAA	114	ASP	11.5788	1.5704	21.5873
	AAAA	115	VAL	0.8933	0.6941	1.1589
20	AAAA	116	TYR	5.1843	0.0006	7.7761
20	AAAA	117	LYS	7.1256	0.9679	12.0517
	AAAA	118	VAL	0.0000	0.0000	0.0000
	AAAA	119	ILE	1.4302	0.0000	2.8604
	AAAA	120	TYR	0.0104	0.0005	0.0153
25	AAAA	121	TYR	2.8600	0.0167	4.2816
	AAAA	122	LYS	3.8739	0.7828	6.3468
	AAAA	123	ASP	11.0893	7.0588	15.1198
	AAAA	124	GLY	13.7649	13.7649	0.0000
	AAAA	125	GLU	8.1492	0.5254	14.2483
30	AAAA	126	ALA	1.3596	0.7744	3.7005
<b>5</b> 0	AAAA	127	LEU	5.0008	0.9822	9.0194
	AAAA	128	LYS	10.8601	0.1501	19.4280
	AAAA	129	TYR	5.7014	3.8333	6.6354
	AAAA	130	TRP	7.7631	0.9621	10.4835
35	AAAA	131	TYR	3.0458	1.1141	4.0116
	AAAA	132	GLU	11.1091	2.1808	18.2518
	AAAA	133	ASN	5.2028	5.3196	5.0859
	AAAA	134	HIS	8.3482	1.2156	13.1032
	AAAA	135	ASN	1.2934	0.3190	2.2679
40	AAAA	136	ILE	2.1274	1.3695	2.8853
, •	AAAA	137	SER	10.0348	7.2335	15.6375
	AAAA	138	ILE	3.6211	1.0099	6.2322
	AAAA	139	THR	16.0640	2.5 <b>8</b> Cპ	34.0420
	AAAA	140	ASN	5.4194	3.6273	7.2114
45	AAAA	141	ALA	0.0000	0.0000	0.0000
	AAAA	142	THR	7.2278	0.4616	16.2495
	AAAA	143	VAL	7.6811	1.4982	15.9250
	AAAA	144	GLU	14.2939	4.1689	22.3939
	AAAA	145	ASP	4.3509	0.0318	8.6701
50	AAAA	146	SER	5.2566	3.1044	9.5609
	AAAA	147	GLY	3.2376	3.2376	0.0000
	AAAA	148	THR	5.2658	0.0995	12.1542
	AAAA	149	TYR	0.2165	0.0000	0.3248
	AAAA	150	TYR	3.8830	0.0000	5.8245
55	AAAA	151	CYS	0.0000	0.0000	0.0000
	AAAA	152	THR	3.7398	0.0010	8.7248

	AAAA	153	GLY	1.0201	1.0201	0.0000
	AAAA	154	LYS	4.0119	0.0425	7.1873
	AAAA	155	VAL	0.4567	0.0000	1.0656
	AAAA	156	TRP	11.1226	3.7204	14.0834
5	AAAA	157	GLN	8.2831	3.3029	12.2673
3	AAAA	158	LEU	13.8927	0.1434	27.6420
	AAAA	159	ASP	9.7733	4.0346	15.5120
		160	TYR	3.4354	2.0054	4.1504
	AAAA	161	GLU	8.2007	5.4400	10.4093
10	AAAA		SER	1.2173	1.8259	0.0002
10	AAAA	162		9.4751	0.3080	16.8088
	AAAA	163	GLU		1.5247	20.8774
	AAAA	164	PRO	9.8187 1.6583	0.0972	3.2194
	AAAA	165	LEU		1.2362	7.2117
	AAAA	166	ASN	4.2239	1.1307	0.0038
15	AAAA	167-	ILE	0.5672	0.0604	21.7538
	AAAA	168	THR	9.3576		
	AAAA	169	VAL	0.5466	0.9510	0.0074
	AAAA	170	ILE	10.6664	1.5666	19.7663
	AAAA	171	LYS	20.0709	14.6286	24.4247
20	AAAA	221	NAG	13.0731	0.0000	13.0731
	AAAA	222	NAG	19.9260	0.0000	19.9260
	AAAA	242	NAG	10.0968	0.0000	10.0968
	AAAA	243	NAG	9.7429	0.0000	9.7429
	AAAA	244	MAN	16.5025	0.0000	16.5025
25	AAAA	250	NAG	16.0048	0.0000 -	16.0048
	AAAA	274	NAG	21.9758	0.0000	21.9758
	AAAA	335	NAG	15.0266	0.0000	15.0266
	AAAA	340	NAG	10.2058	0.0000	10.2058
	AAAA	366	NAG	14.2003	0.0000	14.2003
30	AAAA	367	NAG	21.1043	0.0000	21.1043
	BBBB	4	LYS	21.2711	8.1950	31.7320
	BBBB	5	PRO	0.9327	1.4134	0.2918
	BBBB	6	LYS	13.5721	0.9858	23.6411
	BBBB	7	VAL -	1.5696	2.7468	0.0000
35	BBBB	8	SER	9.0540	1.8158	23.5305
	BBBB	9	LEU	3.7548	4.6164	2.8932
	BBBB	10	ASN	12.3838	0.9742	23.7933
	BBBB	11	PRO	8.3839	0.5771	18.7929
	BBBB	12	PRO	10.2255	2.2114	20.9110
40	BBBB	13	TRP	1.5767	0.1420	2.1505
10	BBBB	14	ASN	3.6856	0.2734	7.0977
	BBBB	15	ARG	1.6517	0.0084	2.5908
	BBBB	16	ILE	1.1539	0.0000	2.3079
	BBBB	17	PHE	0.2627	0.0000	0.4128
45	BBBB	18	LYS	10.5872	3.1464	16.5399
43	BBB8	19	GLY	5.2452	5.2452	0.0000
	8888	20	GLU	3.4004	0.0000	6.1208
	8888	21	ASN	5.3165	3.8893	6.7437
	BBBB	22	VAL	0.3290	0.4639	0.1492
50	BBBB	23	THR	5.3376	0.0419	12.3986
JU	BBBB	23 24	LEU	0.2556	0.0000	0.5112
	BBBB	2 <del>4</del> 25	THR	4.8687	0.0000	11.3603
	8888	25 26	CYS	0.2112	0.2986	0.0364
		20 27	ASN	0.5141	0.1099	0.9184
E E	BBBB	28	GLY	2.2181	2.2181	0.0000
55	BBBB		ASN	10.0991	5.9026	14.2956
	BBBB	29	YON	10.0331	J.3020	17.2000

			•			
	BBBB	30	ASN	8.2629	8.5326	7.9932
	BBBB	31	PHE	13.1098	3.1872	18.7798
	BBBB	32	PHE	3.2118	5.7094	1.7846
	BBBB	33	GLU	9.8599	4.6157	14.0553
5	BBBB	34	VAL	4.2409	3.1111	5.7472
3	8888	35	SER	14.4622	2.1340	39.1186
	BBBB	36	SER	7.0903	1.9980	17.2748
	BBBB	37	THR	0.7246	1.2681	0.0000
	BBBB	38	LYS	8.3435	0.2936	14.7834
10	BBBB	39	TRP	0.0045	0.0000	0.0063
10	BB88	40	PHE	3,0307	0.0013	4.7618
	BBBB	41	HIS	3.2985	0.2952	5.3007
	BBBB	42	ASN	3.9446	4.4215	3.4677
	BBBB	43	GLY	6.4448	6.4448	0.0000
15	BBBB	44	SER	7.9300	1.5277	20.7347
13	888B	45	LEU	14.0360	6.3402	21.7318
	BBBB	46	SER	5.3085	3.4386	9.0482
	BBBB	47	GLU	19.8137	7.9994	29.2651
•	BBBB	48	GLU	6.1811	2.3816	9.2207
20	BBBB	49	THR	10.8045	0.0111	25.1957
20	BBBB	50	ASN	3.7967	1.0050	6.5885
	BBBB	51	SER	1.0119	0.0000	3.0357
	BBBB	52	SER	2.8985	0.0010	8.6934
		53	LEU	2.8664	0.0001	5.7327
05	8888 8888	54	ASN	7.0968	3.9693 ·	10.2244
25.	888B	55	ILE	2.0503	1.4906	2.6099
	BBBB	56	VAL	11.3539	1.8189	24.0671
	BBBB	57	ASN	9.2620	1.0325	17.4916
	BBBB	58	ALA	0.3961	0.4951	0.0000
20	BBBB	59	LYS	13.4689	0.0284	24.2213
30	BBBB	60	PHE	3.3978	0.2767	5.1813
	88 <b>8</b> 8	61	GLU	8.8117	0.1782	15.7185
	BBBB	62	ASP	4.1350	0.0756	8.1943
	8888	63	SER	0.1730	0.0000	0.5191
25	B888	64	GLY	0.0000	0.0000	0.0000
35	8888	65	GLU	6.5484	0.0001	11.7871
	8888	66	TYR	0.7915	0.0000	1.1872
	BBBB	67	LYS	3.2805	0.0000	5.9049
		68	CYS	0.0000	0.0000	0.0000
40	BBBB BBBB	69	GLN	3.8141	0.0000	6.8654
40	88 <b>8</b> 8	70	HIS	0.1609	0.2608	0.094ა
	BBBB	70 71	GLN	10.6127	5.2959	14.8662
	BBBB	72	GLN	8.4010	6.0152	10.3096
	888B	73	VAL	2.9562	2.5768	3.4619
45	8888	74	ASN	7.3147	0.9982	13.6312
43	BBBB	75	GLU	9,4113	4.1701	13.6043
	BBBB	76	SER	0.5684	0.8526	0.0000
	8888	77	GLU	15.8600	1.0254	27.7 <b>278</b>
	888B	77 78	PRO	8.2998	5.0247	12.6666
50	888B	76 79	VAL	5.5759	1.3782	11.1729
50		80	TYR	6.2317	1.9484	8.3734
	8888 8888	81	LEU	0.2490	0.0005	0.4975
	888B	82	GLU	5.8300	0.0000	10.4940
	8888	83	VAL	1.5904	2.7832	0.0000
55	8888	84	PHE	2.7220	0.7033	3.8756
55	BBBB	85	SER	10.7069	5.7965	20.527
	2000	-				

	BBBB	86	ASP	5.9874	2.1888	9.7860
	BBBB	87	TRP	9,1171	0.3262	12.6335 `
	BBBB	88	LEU	0.0289	0.0578	0.0000
	BBBB	89	LEU	0.0888	0.0000	0.1776
5	BBBB	90	LEU	0.0000	0.0000	0.0000
_	BBBB	91	GLN	0.2626	0.0000	0.4726
	BBBB	92	ALA	0.0481	0.0399	0.0813
	888B	93	SER	4.6672	2.9572	8.0872
	BBBB	94	ALA	8.7256	1.3164	38.3623
10	BBBB	95	GLU	7.1764	1.5358	11.6889
	BBBB	96	VAL	12.6418	4.7054	23.2237
	BBBB	97	VAL	1.4061	1.1339	1.7691
	BBBB	98	MET	11.9430	0.2070	23.6789
	BBBB	99	GLU	7.2607	4.6466	9.3520
15	BBBB	100	GLY	5.1244	5.1244	0.0000
15	BBBB	101	GLN	4.0221	0.0000	7.2398
	BBBB	102	PRO	7.3498	1.5529	15.0790
	BBBB	103	LEU	0.0071	0.0138	0.0004
	BBBB	104	PHE	6.2937	0.0007	9.8898
20	BBBB	105	LEU	0.0567	0.0603	0.0531
20	BBBB	106	ARG	2.3037	0.0000	3.6201
	BBBB	107	CYS	0.8127	1.2098	0.0186
	BBBB	108	HIS	1.1982	0.2627	1.8218
	BBBB	109	GLY	1.2842	1.2842	0.0000
25	BBBB	110	TRP	4.4804	0.3255	6.1423
23	BBBB	111	ARG	14,4479	6.9241	18.7472
	BBBB	112	ASN	12.2860	3.9115	20.6605
	888B	113	TRP	7.0297	3.4023	8.4806
	BBBB	114	ASP	11.5554	1.8648	21.2461
30	BBBB	115	VAL	0.8700	0.6238	1.1983
30	BBBB	116	TYR	5.8899	0.0000	8.8349
	BBBB	117	LYS	11.0072	0.9540	19.0498
	BBBB	118	VAL	0.0000	0.0000	0.0000
	8888	119	ILE	4.7824	0.0000	9.5649
35	BBBB	120	TYR	0.0292	0.0003	0.0436
33	BBBB	121	TYR	3.6258	0.0127	5.4323
	BBBB	122	LYS	3.8173	0.8234	6.2125
	BBBB	123	ASP	11.1350	7.1239	15.1460
		123	GLY	13.9353	13.9353	0.0000
40	8888 8888	125	GLU	13.4298	0.5494	23.7341
40	BBBB	126	ALA	15.0233	5.4413	53.3510
	BBBB	127	LEU	9.2699	5.9635	12.5762
	BBBB		LYS	11.6633	1.8096	19.5508
		128	TYR	10.3608	5.2815	12.9005
45	BBBB	129 130	TRP	8.0170	1.0064	10.8213
45	BBBB			11.7311	1.0656	17.0638
	BBBB	131	TYR	12.8760	2.2402	21.3846
	BBBB	132	GLU ASN	5.2983	5.3131	5.2835
	BBBB	133				12.3886
50	BBBB	134	HIS ASN	7.9203	1.2177	2.2995
50	BBBB	135		1.3098	0.3200	
	BBBB	136	ILE	2.0145	1.4037	2.6254
	BBBB	137	SER	9.9370	7.1329	15.5453
	BBBB	138	ILE	3.5989	0.9814	6.2165
66	BBBB	139	THR	16.3957	2.4548	34.9836
55	BBBB	140	ASN	6.1076	3.6820	8.5333
	BBBB	141	ALA	0.0000	0.0000	0.0000

-398-

	8888 8888	142 143	THR VAL	6.9409	0.3571	15.7193
	- BBBB	143	GLU	8.0179 13.9749	1.4651	16.7550
	8888	145	ASP	4.2546	4.2931	21.7203
5	8888	146			0.0236	8.4857
J	8888		SER	5,2200	3.1447	9.3705
		147	GLY	3.2638	3.2638	0.0000
	8888	148	THR	5.2033	0.0855	12.0270
	BBBB	149	TYR	0.2349	0.0000	0.3523
10	BBBB	150	TYR	3.8297	0.0006	5.7443
10	BBBB	151	CYS	0.0001	0.0002	0.0000
	BBBB	152	THR	3.8729	0.01 15	9.0216
	8888	153	GLY	1.0080	1.0080	0.0000
	BBBB	154	LYS	6.2899	0.0456	11.2854
15	BBBB	155	VAL	0.4338	0.0000	1.0121
15	BBBB	156	TRP	10.7002	3.5331	13.6790
	BBBB	157	GLN	13.5388	3.3217	21.7125
	BBBB	158	LEU	13.7581	0.1277	27.3885
	BBBB	159	ASP	13.8236	4.9295	22.7177
20	8888	160	TYR	3.3842	2.5049	3.8239
20	BBBB	161	GLU	12.8172	5.3317	18.8056
	BBBB	162	SER	1.1166	1.6744	0.0011
	BBBB	163	GLU	9.2415	0.1789	16.4915
	BBBB	164	PRO	9.7119	1.5204	20.6339
٥٣	BBBB	165	LEU	1.6353	0.0985	3.1722
25	8888	166	ASN	4.1241	1.1171 -	7.1311
	BBBB	167	ILE	0.5678	1.1351	0.0006
	BBBB	168	THR	9.4957	0.0238	22.1247
	BBBB	169	VAL	0.5214	0.9124	0.0000
20	BBBB	170	ILE	10.7674	1.5460	19.9889
30	BBBB	171	LYS	19.3575	14.1022	23.5617
	BBBB	221	NAG	13.1653	0.0000	13.1653
	BBBB	222	NAG	20.0638	0.0000	20.0638
	BBBB	242	NAG	5.8770	0.0000	5.8770
25	BBBB	243	NAG	6.5918	0.0000	6.5918
35	BBBB	244	MAN	16.4886	0.0000	16.4886
	BBBB	250	NAG	16.1285	0.0000	16.1285
	BBBB	274	NAG	20.2170	0.0000	20.2170
	BBBB	335	NAG	14.9859	0.0000	14.9859
40	BBBB	340	NAG	17.5037	0.0000	17.5037
40	BBBB	366	NAG	14.5337	0.0000	14.5337
	BBBB	367	NAG	21.0686	0.0000	21.0686
	DDDD	4	LYS	22.4057	10.8330	31.6640
	DDDD	5	PRO	1.1546	1.4746	0.7280
AE	DDDD	6	LYS	17.0122	1.1737	29.6830
45	DDDD	7	VAL	1.5813	2.7670	0.0004
	DDDD	8	SER	9.0050	1.8942	23.2265
	DDDD	9	LEU	3.6933	4.6049	2.7818
	DDDD	10	ASN	12.3091	1.0020	23.6161
50	DDDD	11	PRO	8.3171	0.5504	18.6727
50	DDDD	12	PRO	9.9864	2.1032	20.4973
	DDDD	13	TRP	1.5517	0.0931	2.1352
	DDDD	14	ASN	3.3780	0.3110	6.4451
	DDDD	15	ARG	1.6343	0.0116	2.5615
<i>E E</i>	DDDD	16	ILE	1.1547	0.0005	2.3088
55	DDDD	17	PHE	0.2492	0.0000	0.3916
	סססס	18	LYS	4.6732	2.0544	6.7683

	DDDD	19	GLY	3.1162	3.1162	0.0000
	DDDD	20	GLU	3.5200	0.0000	6.3359
	DDDD	21	ASN	5.4287	3.8849	6.9725
	DDDD	22	VAL	0.3155	0.4412	0.1479
5	DDDD	23	THR	5.1394	0.0324	11.9489
•	DDDD	24	LEU	0.2366	0.0000	0.4733
	DDDD	25	THR	4.8738	0.0000	11.3721
	DDDD	26	CYS	0.2520	0.3402	0.0757
	DDDD	27	ASN	7.6624	1.9816	13.3432
10	DDDD	28	GLY	7.7316	7.7316	0.0000
	DDDD	29	ASN	17.3095	8.4320	26.1871
	DDDD	30	ASN	14.6001	10.1471	19.0532
	DDDD	31	PHE	18.5570	8.7657	24.1521
	DDDD	32	PHE	7.0815	6.8006	7.2420
15	DDDD	33	GLU	17.2171	4.7180	27.2164
	DDDD	34	VAL	10.0324	3.1007	19.2746
	DDDD	35	SER	14.2871	2.1039	38.6536
	DDDD	36	SER	6.9328	1.7803	17.2376
	DDDD	37	THR	0.7026	1.2295	0.0000
20	DDDD	38	LYS	8.3451	0.3160	14.7683
	DDDD	39	TRP	0.0041	0.0023	0.0049
	DDDD	40	PHE	2.9900	0.0009	4.6980
	DDDD	41	HIS	3.3768	0.3997	5.3616
	DDDD	42	ASN	6.4948	7.0880	5.9016
25	DDDD	43	GLY	9.5817	9.5817 ·	0.0000
	DDDD	44	SER	12.6350	2.9429	32.0194
	DDDD	45	LEU	14.2578	6.4935	22.0220
	DDDD	46	SER	5.6757	3.8029	9.4212
	DDDD	47	GLU	19.9087	7.8667	29.5423
30	DDDD	48	GLU	6.0890	2.3899	9.0482
	DDDD	49	THR	10.8314	0.0116	25.2577
	DDDD	50	ASN	3.8373	0.9946	6.6800
	DDDD	51	SER	0.9841	0.0000	2.9524
	DDDD	52	SER	2.8765	0.0001	8.6293
35	DDDD	53	LEU	2.8376	0.0187	5.6565
	DDDD	54	ASN	7.0382	3.8726	10.2037
	DDDD	55	ILE	2.0467	1.4442	2.6492
•	DDDD	56	VAL	11.5050	1.8629	24.3611
	DDDD	57	ASN	8.8180	1.0298	16.6062
40	DDDD	58	ALA	0.2350	0.2934	0.0018
	DDDD	59	LYS	13.6844	0.0264	24.6108
	DDDD	60	PHE	2.6066	0.0006	4.0957
	DDDD	61	GLU	8.6110	0.1659	15.3671
	DDDD	62	ASP	4.2057	0.0884	8.3230
45	DDDD	63	SER	0.1340	0.0000	0.4019
	DDDD	64	GLY	0.0349	0.0349	0.0000
	DDDD	65	GLU	8.1888	0.0852	14.6716
	DDDD	66	TYR	0.7677	0.0000	1.1516
	DDDD	67	LYS	3.2893	0.0000	5.9208
50	DDDD	68	CYS	0.0005	0.0000	0.0014
	DDDD	69	GLN	3.8578	0.0000	6.9441
	DDDD	70	HIS	2.2626	0.2237	3.6218
	DDDD	71	GLN	15.3304	6.1240	22.6955
	DDDD	72	GLN	18.9257	6.3446	28.9906
55	DDDD	73	VAL	6.4935	2.6517	11.6159
	DDDD	74	ASN	7.2861	0.8315	13.7407

	DDDD	75	GLU	9.5469	4.3906	13.6720
	DDDD	76	SER	0.4742	0.7107	0.0011
	DDDD	77	GLU	16.0719	0.9787	28.1465
	DDDD	78	PRO	8.1673	5.2859	12.0091
5	DDDD	79	VAL	5.7531	1.2596	11.7443
J	DDDD	80	TYR	6.8446	2.1690	9.1823
	DDDD	81	LEU	0.2183	0.0000	0.4367
	DDDD	82	GLU	5.8647	0.0374	10.5265
	DDDD	83	VAL	1.5404	2.6954	0.0005
10	DDDD	84	PHE	2.7805	0.6706	3.9861
10	DDDD	85	SER	6.8439	5.9428	8.6459
	DDDD	86	ASP	6.0109	2.1275	9.8943
	DDDD	87	TRP	4.6976	0.2328	6.4835
	DDDD	88	LEU	0.0296	0.0530	0.0062
15	DDDD	89	LEU	0.0803	0.0002	0.1605
13	DDDD	90	LEU	0.0000	0.0000	0.0000
	DDDD	91	GLN	0.2460	0.0003	0.4426
	DDDD	92	ALA	0.0626	0.0754	0.0113
	DOOD	93	SER	4.5712	2.8665	7.9807
20	aaaa	94	ALA	8.7178	1.3188	38.3138
20	DDDD	95	GLU	7.2886	1.5976	11.8415
	DDDD	96	VAL	12.8114	4.6767	23.6578
	DDDD	97	VAL	1.4641	1.1764	1.8477
	DDDD	98	MET	13.4393	0.1457	26.7329
25	DDDD	99	GLU	7.1147	4.7251	9.0264
23	DDDD	100	GLY	5.3684	5.3684	0.0000
	DDDD	101	GLN	9.8859	0.0000	17.7946
	DDDD	102	PRO	9.5952	1.6262	20.2206
	DDDD	103	LEU	0.0075	0.0150	0.0000
30	DDDD	104	PHE	6.3221	0.0000	9.9347
50	DDDD	105	LEU	0.0690	0.0712	0.0667
	DDDD	106	ARG	2.3233	0.0001	3.6509
	DDDD	107	CYS	0.8061	1.2091	0.0000
	DDDD	108	HIS	1.1851	0.2808	1.7880
35	DDDD	109	GLY	1.2333	1.2333	0.0000
33	DDDD	110	TRP	0.7404	0.3219	0.9078
	DDDD	111	ARG	7.9699	6.6124	8.7456
	DDDD	112	ASN	12.5024	3.9088	21.0960
	DDDD	113	TRP	2.0923	3.4514	1.5487
40	DDDD	114	ASP	11.6891	1.9841	21.3940
40	DDDD	115	VAL	0.8907	0.6666	1.1894
	DDDD	116	TYR	3.5406	0.0000	5.3109
	DDDD	117	LYS	7.4915	0.9137	12.7537
	DDDD	118	VAL	0.0000	0.0000	0.0000
45	DDDD	119	ILE	1.5354	0.0000	3.0708
45	DDDD	120	TYR	0.0227	0.0000	0.0341
	DDDD	121	TYR	3.0000	0.0000	4.5000
	DDDD	122	LYS	3.8497	0.8215	6.2723
	DDDD	123	ASP	11.0185	7.2080	14.8291
50	DDDD	124	GLY	13.8186	13.8186	0.0000
55	DDDD	125	GLU	7.1969	0.5597	12.5066
	DOOD	126	ALA	1.6231	0.9637	4.2606
	DDDD	127	LEU	5.5580	1.1317	9.9843
	DDDD		LYS	11.0326	0.1803	19.7145
55	DDDD		TYR	6.0662	4.5993	6.7997
	DDDD		TRP	<b>6.9751</b> .	0.9821	9.3722

	DDDD	131	TYR	3.2844	1.1357	4.3587
	DDDD	132	GLU	10.5294	2.1545	17.2294
	DDDD	133	ASN	5.3145	5.3786	5.2503
	DDDD	134	HIS	8.2621	1.1783	12.9846
5	DDDD	135	ASN	1.2924	0.3403	2.2445
	DDDD	136	ILE	2.0846	1.3968	2.7725
	DDDD	137	SER	10.0460	7.2958	15.5465
	DDDD	138	ILE	3.5719	0.9619	6.1819
	DDDD	139	THR	16.0437	2.5113	34.0868
10	DDDD	140	ASN	6.1043	3.6342	8.5744
	DDDD	141	ALA	0.0006	0.0000	0.0028
	DDDD	142	THR	7.0414	0.4613	15.8150
	DDDD	143	VAL	7.7914	1.5021	16.1770
	DDDD	144	GLU	13.9850	4.2384	21.7824
15	DDDD	145	ASP	4.1793	0.0265	8.3322
	DDDD	146	SER	5.2665	3.1409	9.5178
	DDDD	147	GLY	3.2916	3.2916	0.0000
	DDDD	148	THR	5.1835	0.0792	11.9891
	DDDD	149	TYR	0.2058	0.0000	0.3087
20	DDDD	150	TYR	3.8607	0.0000	5.7910
	DDDD	151	CYS	0.0000	0.0000	0.0000
	DDDD	152	THR	3.9195	0.0065	9.1368
	DDDD	153	GLY	1.0864	1.0864	0.0000
	DDDD	154	LYS	5.0786	0.0302	9.1174
25	DDDD	155	VAL	0.4195	0.0000	0.9789
	DDDD	156	TRP	1.3921	2.1135	1.1036
	DDDD	157	GLN	5.1 <b>05</b> 0	3.3675	6.4950
	DDDD	158	LEU	13.2526	0.1201	26.3851
	DDDD	159	ASP	7.9559	2.3964	13.5153
30	DDDD	160	TYR	2.2863	2.2919	2.2835
	DDDD	161	GLU	10.7234	4.9235	15.3634
	DDDD	162	SER	1.2506	1.8759	0.0000
	DDDD	163	GLU	9.3458	0.2040	16.6593
	DDDD	164	PRO	9.8122	1.5651	20.8083
35	DDDD	165	LEU	1.6668	0.0989	3.2347
	DDDD	166	ASN	4.0892	1.1470	7.0314
	DDDD	167	ILE	0.5690	1.1374	0.0006
	DDDD	168	THR	9.4203	0.0533	21.9098
40	DDDD	169	VAL	0.5492	0.9611	0.0000
40	DDDD	170	ILE	10.5373	1.6298	19.4449
	DDDD	171	LYS	19.4334	14.2443	23.5846
	DDDD	221	NAG	12.4351	0.0000	12.4351
	DDDD	222	NAG	14.2041	0.0000	14.2041
	DDDD	242	NAG	9.7024	0.0000	9.7024
45	DDDD	243	NAG	9.7925	0.0000	9.7925
	DDDD	244	MAN	16.4248	0.0000	16.4248
	DDDD	250	NAG	15.9655	0.0000	15.9655
	DDDD	274	NAG	21.7485	0.0000	21.7485
<b>50</b>	DDDD	335	NAG	15.0635	0.0000	15.0635
50	DDDD	340	NAG	17.6569	0.0000	17.6569
	DDDD	366	NAG	14.5792	0.0000	14.5792
	DDDD	367	NAG	20.8687	0.0000	20.8687
	EEEE	4	LYS	22.3558	10.9740	31.4612
		5	PRO	1.1163	1.4301	0.6978
55	EEEE	6	LYS	16.9326	1.2182	29.5041
	EEEE	7	VAL	1.5370	2.6897	0.0000

	EEEE	8	SER	9.0470	1.8198	23.5014
	EEEE	9	LEU	3.7362	4.7200	2.7524
	EEEE	10	ASN	12.0492	0.9478	23.1505
_	EEEE	11	PRO	8.3799	0.5532	18.8156
5	EEEE	12	PRO	9.8266	2.0198	20.2356
	EEEE	13	TRP	1.5826	0.0955	2.1775
	EEEE	14	ASN	3.6101	0.2979	6.9223
	EEEE	15	ARG	1.6218	0.0098	2.5429
	EEEE	16	ILE	1.1456	0.0000	2.2912
10	EEEE	17	PHE	0.2563	0.0000	0.4027
	EEEE	18	LYS	10.9294	3.6992	16.7135
	EEEE	19	GLY	5.6751	5.6751	0.0000
	EEEE	20	GLU	3.4651	0.0024	6.2352
	EEEE	21	ASN	5.3587	3.9397	6.7777
15	EEEE	22	VAL.	0.3206	0.4678	0.1243
	EEEE	23	THR	5.2106	0.0240	12.1261
	EEEE	24	LEU	0.2668	0.0000	0.5335
	EEEE	25	THR	4.8755	0.0000	11.3763
	EEEE	26	CYS	0.2422	0.3394	0.0477
20	EEEE	27	ASN	7.5792	1.5782	13.5803
	EEEE	28	GLY	7.7171	7.7171	0.0000
	EEEE	29	ASN	17.1451	8.1440	26.1463
	EEEE	30	ASN	14.2079	9.6254	18.7903
-	EEEE	31	PHE	18.7547	8.6665	
25	EEEE	32	PHE	7.2539	7.0102	24.5194
	EEEE	33	GLU	17.0855	4.7908	7.3931
	EEEE	34	VAL	10.0735	3.1424	26.9213
	EEEE	35	SER	13.8902	2.0792	19.3149
	EEEE	36	SER	6.8523	1.7904	37.5120
30	EEEE	37	THR	0.6763	1.1836	16.9760
	EEEE	38	LYS	8.3619	0.3108	0.0000
	EEEE	39	TRP	0.0083	0.0020	14.8028
	EEEE	40	PHE	3.0042	0.0000	0.0108
	EEEE	41	HIS	3.3299	0.3808	4.7209
35	EEEE	42	ASN	6.3452	7.0674	5.2960
	EEEE	43	GLY	9.6662	9.6662	5.6231
	EEEE	44	SER	12.6323	3.0497	0.0000
	EEEE	45	LEU	14.2883	6.9452	31.7975
	EEEE	46	J.JR	5.9546		21.6315
40	EEEE	47	GLU	19.8778	3.8685	10.1268
	EEEE	48	GLU	6.2775	7.9851	29.3920
	FFFF	49	THR		2.2956	9.4630
	EEEE	<del>5</del> 0	ASN	11.1492	0.0819	25.9055
	EEEE	51	SER	3.8263	0.9910	6.6616
45	EEEE	52	SER	0.9846	0.0000	2.9539
	EEEE	53	LEU	2.8049	0.0006	8.4134
	EEEE	54		2.6766	0.0083	5.3450
	EEEE	5 <del>4</del> 55	ASN	7.1063	3.8883	10.3243
	EEEE		ILE	2.1074	1.5164	2.6984
50	EEEE	56 57	VAL	11.4388	1.7734	24.3260
J0		57 59	ASN	8.9664	1.0480	16.8848
	EEEE EEEE	58	ALA	0.3426	0.4045	0.0949
		59 60	LYS	13.5640	0.0175	24.4012
	EEEE	60	PHE	3.4104	0.0051	5.3562
55	EEEE	61	GLU	8.6064	0.1863	15.3424
<i>JJ</i>	EEEE	62	ASP	4.2246	0.0962	8.3531
	EEEE	63	SER	0.1134	0.0000	0.3402

	EEEE	64	GLY	0.0266	0.0266	0.0000
	EEEE	65	GLU	4.0549	0.0880	7.2284
	EEEE	66	TYR	0.7832	0.0000	1.1748
	EEEE	67	LYS	3.2565	0.0000	5.8617
5	EEEE	68	CYS	0.0003	0.0005	0.0000
	EEEE	69	GLN	3.8454	0.0000	6.9217
	EEEE	70	HIS	2.2450	0.2224	3.5934
	EEEE	71	GLN	5.9169	3.6396	7.7387
	EEEE	72	GLN	7.4965	6.0264	8.6726
10	EEEE	73	VAL	6.4019	2.4812	11.6294
	EEEE	74	ASN	7.3226	0.8649	13.7804
	EEEE	75	GLU	9.5795	4.4019	13.7216
	EEEE	76	SER	0.7013	1.0519	0.0000
	EEEE	77	GLU	13.4227	1.1013	
15	EEEE	78	PRO	2.4705	1.5274	23.2799
	EEEE	79	VAL	5.5768	0.7997	3.7280
	EEEE	80	TYR	3.6523	1.2328	11.9463
	EEEE	81	LEU	0.2451		4.8621
	EEEE	82	GLU	5.5763	0.0000	0.4902
20	EEEE	83	VAL		0.0256	10.0168
20	EEEE			1.5663	2.7355	0.0074
	EEEE	84 85	PHE	2.8317	0.6685	4.0678
		85	SER	11.1097	5.8236	21.6819
	EEEE	86	ASP	6.3216	2.7103	9.9328
25	EEEE	87	TRP	9.2509	0.2339	12.8578
25	EEEE	88	LEU	0.0596	0.1001	0.0191
	EEEE	89	LEU	0.1011	0.0000	0.2022
	EEEE	90	LEU	0.0000	0.0000	0.0000
	EEEE	91	GLN	0.2558	0.0000	0.4604
••	EEEE	92	ALA	0.0564	0.0519	0.0745
30	EEEE	93	SER	4.5837	2.9367	7.8777
	EEEE	94	ALA	8.3906	1.2888	36.7978
	EEEE	95	GLU	4.4 <b>29</b> 6	1.5357	6.7447
	EEEE	96	VAL	4.3010	4.6742	3.8035
	EEEE .	97	VAL	1.4250	1.0740	1.8929
35	EEEE	98	MET	13.5431	0.2108	26.8754
	EEEE	99	GLU	7.1778	4.7822	9.0943
	EEEE	100	GLY	5.0685	5.0685	0.0000
	EEEE	101	GLN	9.8626	0.0125	17.7427
	EEEE	102	PRO	9.4878	1.6105	19.9908
40	EEEE	103	LEU	0.0128	0.0246	0.0009
	EEEE	104	PHE	6.2895	0.0000	9.8835
	EEEE	105	LEU	0.0574	0.0715	0.0432
	EEEE	106	ARG	2.3284	0.0000	3.6589
	EEEE	107	CYS	0.7794	1.1691	0.0000
45	EEEE	108	HIS	1.2031	0.2846	1.8155
	EEEE	109	GLY	1.3076	1.3076	0.0000
	EEEE	110	TRP	4.3507	0.3127	5.9659
	EEEE	111	ARG	14.5626	6.7438	19.0305
	EEEE	112	ASN	12.6107	3.8715	
50	EEEE	113	TRP	7.0410	3.3592	21.3499
-	EEEE	114	ASP	11.4765		8.5138
	EEEE	115	VAL		1.9258	21.0271
	EEEE	116	TYR	0.8593	0.6604	1.1244
	EEEE	117		5.8929	0.0005	8.8392
55	EEEE		LYS	11.3051	0.9380	19.5988
55	EEEE	118 119	VAL	0.0000	0.0000	0.0000
	CEEE	119	ILE	4.8820	0.0000	9.7641

	EEEE	120	TYR	0.0103	0.0000	0.0154
	EEEE	121	TYR	3.6542	0.0005	5.4811
	EEEE	122	LYS	3.7815	0.6097	6.3190
_	EEEE	123	ASP	10.9462	6.9829	14.9095
5	EEEE	124	GLY	13.7762	13.7762	0.0000
	EEEE	125	GLU	13.1766	0.5548	23.2741
	EEEE	126	ALA	14.6424	5.3245	51.9143
	EEEE	127	LEU	9.2224	5.9305	12.5143
	EEEE	128	LYS	11.5329	1.8633	19.2686
10	EEEE	129	TYR	10.3194	5.0683	12.9449
	EEEE	130	TRP	8.0715	0.9722	10.9112
	EEEE	131	TYR	11.8508	1.0518	17.2503
	EEEE	132	GLU	12.7984	2.2087	21.2701
	EEEE	133	ASN	5.2222	5.2458	5.1985
15	EEEE	134	HIS	8.275	1.2222	12.9775
	EEEE	135	ASN	1.3104	0.3410	2.2798
	EEEE	136	ILE	2.0064	1.3737	
	EEEE	137	SER	10.1799	7.2553	2.6391 16.0292
	EEEE	138	ILE	3.5424	0.9990	
20	EEEE	139	THR	16.1230	2.4880	6.0858
	EEEE	140	ASN	6.0914		34.3029
	EEEE	141	ALA	0.0000	3.7069	8.4760
	EEEE	142	THR		0.0000	0.0000
	EEEE	143	VAL	7.1532	0.3267	16.2552
25	EEEE	144	GLU	4.0502	1.4721	7.4876
23	EEEE	145		14.1982	4.3093	22.1094
	EEEE	146	ASP	4.2616	0.0294	8.4938
	EEEE		SER	5.0852	3.1109	9.0339
	EEEE	147	GLY	3.2633	3.2633	0.0000
30		148	THR	5.3711	0.0808	12.4248
30	EEEE	149	TYR	0.2123	0.0000	0.3185
	EEEE	150	TYR	3.8241	0.0000	5.7362
	EEEE	151	CYS	0.0000	0.0000	0.0000
	EEEE	152	THR	3.8973	0.0053	9.0866
35	EEEE	153	GLY	1.0506	1.0506	0.0000
33	EEEE	154	LYS	6.3259	0.0465	11.3493
	EEEE	155	VAL	0.4347	0.0000	1.0143
	EEEE	156	TRP	10.7736	3.6761	13.6126
	EEEE	157	GLN	13.4826	3.3463	21.5916
40	EEEE	158	LEU	13.9288	0.1999	27.6578
40	EEEE	159	ASP	14.3643	5.1303	23.5982
	EEEE	160	TYR	3.4607	2.4956	3.9432
	EEEE	161	GLU	12.5195	4.7567	18.7297
	EEEE	162	SER	1.0778	1.6166	0.0000
4.5	EEEE	163	GLU	9.3641	0.1874	16.7054
45	EEEE	164	PRO	9.7812	1.5531	20.7519
	EEEE	165	LEU	1.6355	0.0916	3.1794
	EEEE	166	ASN	3.8982	1.0603	6.7362
	EEEE	167	ILE	0.5697	1.1379	0.0016
	EEEE	168	THR	2.3606	0.0217	5.4790
50	EEEE	169	VAL	0.0074	0.0129	0.0000
	EEEE	170	ILE	2.2300	0.0089	4.4512
	EEEE	171	LYS	14.7618	13.0272	16.1495
	EEEE	221	NAG	12.9978	0.0000	12.9978
	EEEE	222	NAG	20.1629	0.0000	20.1629
55	EEEE	242	NAG	8.4007	0.0000	8.4007
	EEEE	243	NAG	8.4488	0.0000	8.4488
				J		J. TTUU

-405-

	EEEE	244	MAN .	16.3142	0.0000	16,3142
	EEEE	250	NAG	15.9751	0.0000	15.9754
	EEEE	274	NAG	18.4789	0.0000	18,4789
	EEEE	335	NAG	14.8589	0.0000	14.8589
5	EEEE	340	NAG	17.7265	0.0000	17.7265
	EEEE	366	NAG	11.7893	0.0000	11.7893
•	EEEE	367	NAG	18 5598	0.0000	18 5509

Table 10. PhFc $\epsilon$ RI $\alpha_{1-172}$ , Form T2, residue exposure

>>> coordinate set= pent74_11c1.pdb

	segid	resid	resname	access	access-main	access-side
		4	LYS	22.5230	10.8738	31.8424
5	CCCC	5	PRO	1.1416	1.5686	0.5722
	CCCC	6	LYS	17.1986	1.4144	29.8259
	CCCC	7	VAL	1.6270	2.8202	0.0362
		8	SER	8.6366	1.9053	22.0990
	CCCC	9	LEU	4.4395	5.4841	3.3949
10	CCCC	10	ASN	12.0444	0.9261	23.1626
	CCCC	11	PRO	7.7510	0.4778	17.4486
	CCCC	12	PRO	10.0046	2.2549	20.3375
	CCCC	13	TRP	1.5672	0.1129	2.1488
	CCCC	14	ASN	3.3834	0.3515	6.4153
15	CCCC	15	ARG	1.7214	0.0000	2.7051
	CCCC	16	ILE	0.9799	0.0000	1.9599
	CCCC	17	PHE	0.2972	0.0000	0.4670
	CCCC	18	LYS	11.0480	3.8504	16. <b>8061</b>
20	CCCC	19	GLY	5.6439	5.6439	0.0000
20		20	GLU	3.6350	0.0352	6.5149
		21	ASN	5.3939	4.1927	6.5951
		22	VAL	0.2954	0.4493	0.0902
		23	THR	5.4708	0.0934	12.6405
25		24	LEU	0.4978	0.0000	0.9957
25		25	THR	5.1976	0.0006	12.1271
		26	CYS	0.3073	0.3299	0.2621
	CCCC		ASN	8.5100	1.3260	15.6940
		28	GLY	6.8597	6.8597	0.0000
20		29	ASN	17.2073	7.8659	26.5486
30		30	ASN	14.4090	9.6919	19.1261
		31	PHE	18.6560	9.4593	23.9112
		\$2	PHE	7.3970	6.8547	7.7068
		33	GLU	17.4505	4.8495	27.5314
35		34	VAL	10.1697	3.7420	18.7399
33		35	SER	14.6634	2.2968	39.3 <del>96</del> 5
		36	SER	7.1609	1.9487	17.5852
		37	THR	0.7165	1.2539	0.0000
		38	LYS	8.8073	0.3430	15.5788
40		39	TRP	0.0048	0.0169	0.0000
<del>-1</del> 0		40 41	PHE	3.0629	0.0000	4.8131
		41 42	HIS	3.2953	0.2185	5.3465
	CCCC		ASN	6.4333	7.3988	5.4678
	CCCC		GLY	8.7787	8.7787	0.0000
45	CCCC		SER	12.5780	3.2206	31.2928
75	CCCC		LEU	14.3835	6.5311	22.2359
	CCCC		SER	6.0642	4.1760	9.8407
	CCCC		GLU	19.8848	8.0573	29.3468
	CCCC		GLU	5.7325	2.1429	8.6042
50	CCCC		THR	11.1779	0.0000	26.0818
J <b>U</b>	CCCC		ASN	3.7291	1.0808	6.3774
		J 1	SER	1.1927	0.0000	3.5780

	CCCC 52	SER	2.7289	0.0000	8.1866
	CCCC 53	LEU	2.8602	0.0189	5.7014
	CCCC 54	ASN	7.0896	4.0346	10.1446
	CCCC 55	ILE	1.9722	1.4947	2.4497
5	CCCC 56	VAL	11.4466	1.8119	24.2929
	CCCC 57	ASN	9.2079	1.1203	17.2954
	CCCC 58	ALA	0.2682	0.3352	0.0000
	CCCC 59	LYS	13.5663	0.0799	24.3554
	CCCC 60	PHE	4.2653	0.0614	6.6675
10	CCCC 61	GLU	9.3104	0.1429	16.6444
	CCCC 62	ASP	4.1004	0.0929	8.1079
	CCCC 63	SER	0.1952	0.0000	0.5857
	CCCC 64	GLY	0.0000	0.0000	0.0000
	CCCC 65	GLU	3.3950	0.0904	6.0387
15	CCCC 66	TYR	1.0210	0.0004	1.5313
	CCCC 67	LYS	3.2922	0.0006	5.9255
	CCCC 68	CYS	0.0000	0.0000	0.0000
	CCCC 69	GLN	4.0273	0.0000	7.2491
••	CCCC 70	HIS	2.4293	0.2618	3.8743
20	CCCC 71	GLN	10.1947	6.5416	23.8992
	CCCC 72	GLN	18.7079	6.7237	28.2952
	CCCC 73	VAL	5.9018	2.0768	11.0019
	CCCC 74	ASN	7.6674	1.2523	14.0824
0.5	CCCC 75	GLU	9.5618	4.3436	13.7363
25	CCCC 76	SER	0.7453	1.1107	0.0146
	CCCC 77	GLU	13.4902	1.2113	23.3134
	CCCC 78	PRO	3.7570	2.4424	5.5097
	CCCC 79	VAL	6.2786	1.0035	13.3121
00	CCCC 80	TYR	4.8276	1.6806	6.4011
30	CCCC 81	LEU	0.4499	0.0000	0.8998
	CCCC 82	GLU	6.0083	0.0302	10.7907
	CCCC 83	VAL	1.5038	2.6317	0.0000
	CCCC 84	PHE	2.9396	0.6034	4.2746
25 /	CCCC 85	SER	11.0379	5.9825	21.1488
35 ′	CCCC 86	ASP	6.6954	2.8722	10.5186
	CCCC 87	TRP	5.7551	0.2523	7.9563
	CCCC 88	LEU	0.0496	0.0992	0.0000
	CCCC 89	LEU	0.0722	0.0000	0.1444
40	CCCC 90	LEU	0.0039	0.0006	0.0071
40	CCCC 91	GLN	0.2715	0.0000	0.4886
	CCCC 92	ALA	0.1064	0.1238	0.0367
	CCCC 93	SER	4.5560	3.0073	7.6533
	CCCC 94	ALA	8.2925	1.3979	35.8708
15	CCCC 95	GLU	5.1869	1.5220	8.1188
45	CCCC 96	VAL	5.3247	4.5540	6.3524
	CCCC 97	VAL	1.5905	0.9728	2.4141
	CCCC 98	MET	14.3166	0.0743	28.5590
	CCCC 99	GLU	7.0891	5.0739	8.7013
50	CCCC 100	GLY	5.1879	5.1879	0.0000
50	CCCC 101	GLN	9.5976	0.0133	17.2651
	CCCC 102	PRO	9.4229	1.5439	19.9284
	CCCC 103	LEU	0.0333	0.0371	0.0295
	CCCC 104	PHE	6.3516	0.0000	9.9811
55	CCCC 105	LEU	0.1059	0.0591	0.1526
55	CCCC 106	ARG	2.2520	0.0000	3.5388
	CCCC 107	CYS	0.6406	0.9609	0.0000

	CCCC 108	HIS	1.1793	0.2252	1.8153
	CCCC 109	GLY	1.3114	1.3114	0.0000
	CCCC 110	TRP	4.6295	0.3368	6.3465
	CCCC 111	ARG	13.1248	6.9961	16.6270
5	CCCC 112	ASN	12.8011	4.3120	21.2901
	CCCC 113	TRP	6.0437	3.3401	7.1251
	CCCC 114	ASP	11.9344	1.8804	21.9884
	CCCC 115	VAL	0.9151	0.7229	1.1714
	CCCC 116	TYR	5.9569	0.0000	8.9354
10	CCCC 117	LYS	11.0444	0.6651	19.3478
	CCCC 118	VAL	0.0000	0.0000	0.0000
	CCCC 119	ILE	4.4790	0.0001	8.9579
	CCCC 120	TYR	0.0043	0.0000`	0.0064
	CCCC 121	TYR	3.7210	0.0085	5.5773
15	CCCC 122	LYS	4.0141	0.9317	6.4800
	CCCC 123	ASP	10.8032	6.5278	15.0786
	CCCC 124	GLY	14.5419	14.5419	0.0000
	CCCC 125	GLU	12.8310	0.4067	22.7705
20	CCCC 126	ALA	14.9558	5.5670	52.5110
20	CCCC 127	LEU	9.4777	6.3362	12.6193
	CCCC 128	LYS	11.7644	1.7577	19.7697
	CCCC 129 CCCC 130	TYR	10.4250	4.9480	13.1636
	CCCC 130	TRP	8.2395	1.0761	11.1049
25	CCCC 131	TYR	12.1293	0.8795	17.7543
23	CCCC 132	GLU ASN	12.7495	1.9453	21.3930
	CCCC 134	HIS	5.6282 8.2353	5.4710	5.7854
	CCCC 135	ASN	1.3610	1.4518	12.7576
	CCCC 136	ILE	2.1395	0.3583 1.3206	2.3637
30	CCCC 137	SER	10.0045	7.3132	2.9584
50	CCCC 138	ILE	3.5461	0.8905	15.3872 6.2017
	CCCC 139	THR	15.6326	2.4796	33.1700
	CCCC 140	ASN	6.4183	3.6583	9.1784
	CCCC 141	ALA	0.0002	0.0000	0.0009
35	CCCC 142	THR	7.3418	0.3932	16.6068
	CCCC 143	VAL	5.5574	1.0899	11.5140
	CCCC 144	GLU	14.2578	4.3490	22.1849
	CCCC 145	ASP	4.1649	0.0654	8.2644
	CCCC 146	SER	5.4994	3.9946	8.5092
40	CCCC 147	GLY	2.9610	2.9610	0.0000
	CCCC 148	THR	5.8295	0.0862	13.4873
	CCCC 149	TYR	0.2839	0.0098	0.4210
	CCCC 150	TYR	3.8352	0.0141	5.7458
	CCCC 151	CYS	0.0000	0.0000	0.0000
45	CCCC 152	THR	3.7535	0.0000	8.7581
	CCCC 153	GLY	1.0847	1.0847	0.0000
	CCCC 154	LYS	6.0253	0.0000	10.8456
	CCCC 155	VAL	0.4796	0.0000	1.1192
<b>5</b> 0	CCCC 156	TRP	5.6483	5.3816	5.7550
50	CCCC 157	GLN	13.9764	3.1848	22.6098
	CCCC 158	LEU	9.4587	0.2983	18.6191
	CCCC 159	ASP	14.1094	4.9876	23.2312
	CCCC 160	TYR	2.5046	2.3069	2.6034
55	CCCC 161	GLU	13.4023	4.9331	20.1776
J	CCCC 162	SER	1.0596	1.5893	0.0000
	CCCC 163	GLU	9.9946	0.7061	17.4254

	CCCC 164	PRO	10.2249	1.5777	21.7546
	CCCC 165	LEU	1.6401	0.1628	3.1175
	CCCC 166	ASN	3.3684	1.0069	5.7299
	CCCC 167	ILE	0.5437	1.0633	0.0240
5	CCCC 168	THR	4.2337	0.0946	9.7525
	CCCC 169	VAL	0.1117	0.1954	0.0000
	CCCC 170	ILE	2.4168	0.0906	4.7430
	CCCC 171	LYS	14.4505	13.2729	15.3926
	CCCC 221	NAG	13.3692	0.0000	13.3692
10	CCCC 222	NAG	19.4652	0.0000	19.4652
	CCCC 242	NAG	9.4466	0.0000	9.4466
	CCCC 243	NAG	8.1868	0.0000	8.1868
	CCCC 244	MAN	18.7031	0.0000	18.7031
	CCCC 250	NAG	16.1904	0.0000	16.7031
15	CCCC 274	NAG	21.9195	0.0000	
10	CCCC 335	NAG	15.0294	0.0000	21.9195
	CCCC 340	NAG	17.5228	0.0000	15.0294
	CCCC 366 **	NAG	12.1164		17.5228
	CCCC 367	NAG		0.0000	12.1164
20	AAAA 4	LYS	19.5921 20.9627	0.0000	19.5921
20	AAAA 5	PRO		10.5913	29.2599
	AAAA 6	LYS	1.1603	1.5921	0.5846
	AAAA 7	VAL	16.7967	1.3698	29.1382
	AAAA 8	SER	1.6748	2.8323	0.1316
25	AAAA 9	LEU	8.1802	1.8708	20.7991
23	AAAA 10		4.4389	5.4321	3.4456
	AAAA 11	ASN	12.2932	0.9523	23.6341
	AAAA 12	PRO	7.8292	0.4916	17.6128
		PRO	9.7721	2.2628	19.7845
30		TRP	1.5676	0.0823	2.1617
30	AAAA 14	ASN	3.0526	0.3315	5.7738
	AAAA 15	ARG	1.7626	0.0011	2.7691
	AAAA 16	ILE	0.9627	0.0000	1.9254
	AAAA 17	PHE	0.3249	0.0000	0.5105
35	AAAA 18	LYS	10.8420	3.4841	16.7283
22	AAAA 19	GLY	5.4381	5.4381	0.0000
	AAAA 20	GLU	3.6790	0.0263	6.6011
	AAAA 21	ASN	5.3743	4.2040	6.5445
	AAAA 22	VAL	0.2940	0.4433	0.0951
40	AAAA 23	THR	5.8035	0.1030	13.4041
40	AAAA 24	LEU	0.4614	0.0000	0.9228
	AAAA 25	THR	5.1305	0.0007	11.9 <b>70</b> 4
	AAAA 26	CYS	0.2915	0.3512	0.1723
	AAAA 27	ASN	6.2421	1.5400	10.9443
45	AAAA 28	GLY	6.9474	6.9474	0.0000
45	AAAA 29	ASN	17.1386	8.6715	25.6057
	AAAA 30	ASN	14.4072	9.6995	19.1150
	AAAA 31	PHE	15.4860	6.5595	20.5869
	AAAA 32	PHE	3.7024	5.7813	2.5144
50	AAAA 33	GLU	6.0657	4.8688	7.0232
50	AAAA 34	VAL	5.5276	3.8118	7.8153
	AAAA 35	SER	14.1613	2.3658	37.7522
	AAAA 36	SER	7.1159	1.7815	17.7848
	AAAA 37	THR	0.7225	1.2641	0.0004
<i>EE</i>	AAAA 38	LYS	8.7294	0.3364	15.4439
55	AAAA 39	TRP	0.0092	0.0322	0.0000
	AAAA 40	PHE	3.1015	0.0000	4.8738

	AAAA 41	HIS	3.4263	0.4703	5.3969
	AAAA 42	ASN	6.4271	7.3557	5.4985
	AAAA 43	GLY	8.7869	8.7869	0.0000
	AAAA 44	SER	12.6493	3.0960	31.7559
5	AAAA 45	LEU	14.5777	6.7914	22.3640
	AAAA 46	SER	5.5814	3.9481	8.8482
	AAAA 47	GLU	19.7555	7.9429	29.2055
	AAAA 48	GLU	5.9957	2.0924	9.1182
	AAAA 49	THR	11.1755	0.0000	26.0762
10	AAAA 50	ASN	3.7477	1.0911	6.4042
	AAAA 51	SER	1.1636	0.0000	
	AAAA 52	SER	2.7526	0.0004	3.4907
	AAAA 53	LEU			8.2570
	AAAA 54	ASN	2.9437	0.0016	5.8859
15	AAAA 55	ILE	7.0747	3.8236	10.3258
13			1.9632	1.5156	2.4109
		VAL	11.4314	1.7967	24.2777
		ASN	8.8194	1.1924	16.4463
	AAAA 58	ALA	0.3818	0.4773	0.0000
20	AAAA 59	LYS	14.0268	0.1179	25.1539
20	AAAA 60	PHE	4.2543	0.0600	6.6511
_	AAAA 61	GLU	9.3832	0.1346	16.7820
•	AAAA 62	ASP	4.0523	0.0770	8.0275
	AAAA 63	SER	0.1601	0.0000	0.4802
~~	AAAA 64	GLY	0.0003	0.0003	0.0000
25	AAAA 65	GLU	7.8567	0.0750	14.0821
	AAAA 66	TYR	1.0215	0.0000	1.5322
	AAAA 67	LYS	3.3027	0.0000	5.9449
	AAAA 68	CYS	0.0000	0.0000	0.0000
	AAAA 69	GLN	3.9650	0.0000	7.1371
30	AAAA 70	HIS	1.3538	0.2724	2.0747
	AAAA 71	GLN	16.3949	6.5138	24.2997
	AAAA 72	GLN	18.9827	6.9646	28.5973
	AAAA 73	VAL	4.9867	2.0211	8.9408
	AAAA 74	ASN	7.4791	1.0651	13.8931
35	AAAA 75	GLU	9.6144	4.2579	13.8996
	AAAA 76	SER	0.6674	0.9903	0.0214
	AAAA 77	GLU	15.9242	1.2854	27.6353
	AAAA 78	PRO	8.1677	4.8944	12.5320
•	AAAA 79	VAL	6.4525	1.5909	12.9345
40	AAAA 80	TYR	7.2923	1.8827	9.9971
	AAAA 81	LEU	0.4642	0.0000	0.9283
	AAAA 82	GLU	6.0060	0.0321	10.7852
	AAAA 83	VAL	1.5422	2.6988	
	AAAA 84	PHE	2.9572	0.6545	0.0000
45	AAAA 85	SER	10.8486	6.1560	4.2730
	AAAA 86	ASP			20.2338
	AAAA 87	TRP	6.1844	2.2433	10.1256
	AAAA 88		9.3655	0.2163	13.0252
	AAAA 89	LEU LEU	0.0504	0.1008	0.0000
50	AAAA 90		0.1469	0.0000	0.2937
50		LEU	0.0016	0.0007	0.0025
		GLN	0.2732	0.0066	0.4865
		ALA	0.0432	0.0426	0.0458
	AAAA 93	SER	4.4502	2.9733	7.4040
55	AAAA 94	ALA	8.7362	1.3963	38.0959
55	AAAA 95	GLU	7.1768	1.5655	11.6658
	AAAA 96	VAL	13.5692	4.6624	25.4450

	AAAA 97	VAL	1.5462	0.9380	2.3571
	AAAA _: 98	MET	14.3960	0.0702	28.7219
	AAAA 99	GLU	7.3826	4.6030	9.6063
_	AAAA 100	GLY	4.9867	4.9867	0.0000
5	AAAA 101	GLN	9.6618	0.0164	17.3782
	AAAA 102	PRO	9.4982	1.5257	20.1283
	AAAA 103	LEU	0.0170	0.0095	0.0245
	AAAA 104	PHE	6.3600	0.0000	9.9943
	AAAA 105	LEU	0.0964	0.0678	0.1250
10	AAAA 106	ARG	2.2271	0.0002	3.4997
	AAAA 107	CYS	0.6410	0.9615	0.0000
	AAAA 108	HIS	1.1779	0.2061	1.8257
	AAAA 109	GLY	1.2835	1.2835	0.0000
15	, AAAA 110	TRP	4.3852	0.3446	6.0014
15	AAAA 111	ARG	14.5965	6.9788	18.9495
	AAAA 112	ASN	13.1375	4.4344	21.8406
	AAAA 113 · AAAA 114	TRP	7.1680	3.4865	8.6407
	AAAA 114 AAAA 115	ASP	11.7831	1.8946	21.6716
20		VAL	0.9352	0.7629	1.1650
20	AAAA 116 AAAA 117	TYR	5.3542	0.0000	8.0313
	AAAA 117 AAAA 118	LYS VAL	7.2506	0.7461	12.4542
	AAAA 119	ILE	0.0000 1.6994	0.0000	0.0000
	AAAA 120	TYR		0.0000	3.3988
25	AAAA 121	TYR	0.0315 2.9781	0.0007 0.0007	0.0469
2.3	AAAA 122	LYS	3.9855	0.7635	4.4667
	AAAA 123	ASP	10.6844	6.3101	6.5630
	AAAA 124	GLY	14.6459	14.6459	15.0587
	AAAA 125	GLU	7.8188	0.3898	0.0000 13.7619
30	AAAA 126	ALA	2.0714	1.0926	5.9866
	AAAA 127	LEU	5.8795	1.4447	10.3142
	AAAA 128	LYS	11.0255	0.1820	19.7002
	AAAA 129	TYR	5.6220	4.2110	6.3275
	AAAA 130	TRP	6.9643	1.0858	9.3157
35	AAAA 131	TYR	2.7608	0.9482	3.6671
	AAAA 132	GLU	9.8508	1.9760	16.1507
	AAAA 133	ASN	5.7009	5.5383	5.8635
	AAAA 134	HIS	8.0039	1.5080	12.3344
	AAAA 135	ASN	1.3397	0.3105	2.3689
40	AAAA 136	ILE	2.1821	1.3384	3.0258
	AAAA 137	SER	9.9955	7.3477	15.2912
	AAAA 138	ILE	3.4842	0.8752	6.0933
	AAAA 139	THR	15.7464	2.4744	33.4424
	AAAA 140	ASN	6.4552	3.7317	9.1786
45	AAAA 141	ALA	0.0000	0.0000	0.0000
	AAAA 142	THR	7.4724	0.4042	16.8967
	AAAA 143	VAL	7.7469	1.0561	16.6680
	AAAA 144	GLU	14.1113	4.3219	21.9429
<b>~</b> 0	AAAA 145	ASP	4.3240	0.0500	8.5980
50	AAAA 146	SER	5.4853	4.0599	8.3361
	AAAA 147	GLY	2.8492	2.8492	0.0000
	AAAA 148	THR	5.7830	0.0884	13.3757
	AAAA 149	TYR	0.2720	0.0018	0.4071
~~	AAAA 150	TYR	3.9253	0.0098	5.8831
55	AAAA 151	CYS	0.0000	0.0000	0.0000
	AAAA 152	THR	3.7350	0.0000	8.7151

	AAAA	153	GLY	1.0268	1.0268	0.0000
	AAAA	154	LYS	4.9160	0.0084	8.8421
	AAAA	155	VAL	0.4691	0.0000	1.0946
	AAAA	156	TRP	11.7056	5.3116	14.2632
5	AAAA	157	GLN	9.2515	3.3242	13.9933
	AAAA	158	LEU	13.8847	0.2727	27.4967
	AAAA	159	ASP	9.2336	3.2139	15.2533
	AAAA	160	TYR	3.5492	2.3626	4.1425
	AAAA	161	GLU	11.2704	5.0419	16.2531
10	AAAA	162	SER	1.1125	1.6687	0.0000
	AAAA	163	GLU	9.7709	0.4328	17.2413
	AAAA	164	PRO	10.3588	1.5740	22.0717
	AAAA	165	LEU	1.6439	0.1655	3.1223
	AAAA	166	ASN	4.0686	1.1039	7.0332
15	AAAA	167	ILE	0.5158	1.0240	0.0075
	AAAA	168	THR	10.0323	0.1297	23.2358
	AAAA	169	VAL	0.5330	0.8959	0.0491
	AAAA	170	ILE	10.6523	1.5082	19.7963
	AAAA	171	LYS	20.1585	15.5532	23.8428
20	AAAA	221	NAG	13 2449	0.0000	13.2449
	AAAA	222	NAG	19.9892	0.0000	19.9892
	AAAA	242	NAG	9.9407	0.0000	9.9407
	AAAA	243	NAG	9.4600	0.0000	9.4600
	AAAA	244	MAN	18.6631	0.0000	18.6631
25	AAAA	250	NAG	16.3080	0.0000	16.3080
	AAAA	274	NAG	21.8749	0.0000	21.8749
	AAAA	335	NAG	15.0157	0.0000	15.0157
	AAAA	340	NAG	17.2280	0.0000	17.2280
•	AAAA	366	NAG	14.4545	0.0000	14.4545
30	AAAA	367	NAG	20.9042	0.0000	20.9042
	BBBB	4	LYS	22.4434	10.6722	31.8604
	BBBB	5	PRO	1.1609	1.5819	0.5996
	BBBB	6	LYS	16.5842	1.4102	28.7235
25	BBBB	7	VAL	1.6862	2.8240	0.1692
35	BBBB	8	SER	8.2982	1.8668	21.1609
	BBBB	9	LEU	4.4129	5.4051	3.4206
	BBBB	10	ASN	11.9525	0.9175	22.9875
	BBBB	11	PRO	7.8250	0.4752	17.6248
40	BBBB	12	PRO	10.1980	2.1957	20.8677
40	BBBB	13	TRP	1.5849	0.0977	2.1798
	BBBB	14	ASN	3.3380	0.3318	6.3443
	BBBB	15	ARG	1.7418	0.0000	2.7372
	BBBB	16	ILE	0.9354	0.0001	1.8707
AE	BBBB	17	PHE	0.3221	0.0000	0.5062
45	BBBB	18	LYS	11.1312	3.8205	16.9798
	BBBB	19	GLY	5.3141	5.3141	0.0000
	BBBB	20	GLU	3.5506	0.0401	6.3590
	BBBB	21	ASN	5.3304	4.1079	6.5530
50	BBBB	22	VAL	0.2845	0.4466	0.0683
50	BBBB	23	THR	5.5150	0.0841	12.7561
	BBBB	24	LEU	0.4740	0.0000	0.9480
	8888	25	THR	5.1331	0.0000	11.9772
	BBBB	26	CYS	0.2892	0.3174	0.2327
55	BBBB	27	ASN	6.4305	1.5210	11.3399
JJ	BBBB	28	GLY	7.2421	7.2421	0.0000
	BBBB	29	ASN	17.3886	8.6086	26.1686

	BBBB 30	ASN	14.2633	10.0072	18.5194
	BBBB 31	PHE	18.8528	9.5505	24.1684
	BBBB 32	PHE	6.5037	6.5617	6.4706
	BBBB 33	GLU	12.9342	4.8992	19.3623
5	BBBB 34	VAL	8.3666	3.8085	14.4440
	BBBB 35	SER	14.2536	2.2580	38.2448
	BBBB 36	SER	7.1333	1.8956	17.6087
	BBBB 37	THR	0.7187	1.2577	0.0000
	BBBB 38	LYS	8.8478	0.3137	15.6751
10	BBBB 39	TRP	0.0155	0.0288	0.0102
••	BBBB 40	PHE	3.1021	0.0000	4.8747
	BBBB 41	HIS	3.3964	0.4181	5.3819
	BBBB 42	ASN	4.3570	5.3484	3.3656
	BBBB 43	GLY	8.6389	8.6389	
15	BBBB 44	SER	12.5229	3.2589	0.0000
	BBBB 45	LEU	14.4289	6.6263	31.0508
	BBBB 46	SER	6.1946	4.5349	22.2316
	BBBB 47	GLU	19.7813		9.5141
	BBBB 48	GLU		8.0788	29.1432
20	BBBB 49	THR	5.7938	2.2706	8.6124
20	BBBB 50		11.0771	0.0000	25.8466
		ASN	3.6499	1.0731	6.2267
	BBBB 51 BBBB 52	SER	1.1954	0.0005	3.5851
		SER	2.7282	0.0002	8.1843
25		LEU	2.6801	0.0033	5.3570
23	BBBB 54 BBBB 55	ASN	7.0535	4.0402	10.0668
		ILE	1.9823	1.5180	2.4466
	BBBB 56 BBBB 57	VAL	11.5628	1.8317	24.5377
		ASN	8.8810	1.1220	16.6400
20	BBBB 58	ALA	0.3193	0.3991	0.0000
30	BBBB 59	LYS	13.7310	0.1005	24.6353
	BBBB 60	PHE	4.2410	0.1526	6.5772
	BBBB 61	GLU	9.1821	0.1249	16.4278
	BBBB 62	ASP	4.1444	0.0742	8.2145
25	BBBB 63	SER	0.1404	0.0003	0.4207
35	BBBB 64	GLY	0.0115	0.0115	0.0000
	BBBB 65	GLU	7.8724	0.0613	14.1212
	BBBB 66	TYR	1.0150	0.0106	1.5171
	BBBB 67	LYS	3.3196	0.0000	5.9752
40	BBBB 68	CYS	0.0000	0.0000	0.0000
40	BBBB 69	GLN	4.0029	0.0000	7.2052
	BBBB 70	HIS	1.6317	0.2424	2.5580
	BBBB 71	GLN	13.5234	6.2391	19.3508
	BBBB 72	GLN	13.7415	5.5049	20.3307
4.5	BBBB 73	VAL	3.0796	1.9941	4.5269
45	BBBB 74	ASN	7.4362	0.9858	13.8867
	BBBB 75	GLU	9.6630	4.3598	13.9056
	BBBB 76	SER	0.6085	0.9051	0.0153
	BBBB 77	GLU	15. <b>826</b> 7	1.2423	27.4942
<b>~</b> 0	BBBB 78	PRO	8.2618	4.8501	12.8107
50	BBBB 79	VAL	6.6038	1.6215	13.2470
	BBBB 80	TYR	7.2918	1.9227	9.9763
	BBBB 81	LEU	0.4359	0.0011	0.8708
	BBBB 82	GLU	5.5353	0.0340	9.9364
	BBBB 83	VAL	1.5227	2.6648	0.0000
55	BBBB 84	PHE	2.9287	0.6127	4.2522
	BBBB 85	SER	11.1963	6.1246	21.3396

	BBBB 86	ASP	6.4970	2.8341	10.1599
	BBBB 87	TRP	9.3025	0.2173	12.9366
	BBBB 88	LEU	0.0466	0.0933	0.0000
	BBBB 89	LEU	0.1325	0.0000	0.2650
5	BBBB 90	LEU	0.0000	0.0000	0.0000
	BBBB 91	GLN	0.2/15	0.0001	0.4887
	BBBB 92	ALA	0.1140	0.1208	0.0870
	BBBB 93	SER	4.3701	3.0355	7.0392
	BBBB 94	ALA	8.8274	1.4714	38.2514
10	BBBB 95	GLU	7.1968	1.4526	11.7922
	BBBB 96	VAL	13.4385	4.5929	25.2325
	BBBB 97	VAL	1.5907	0.9613	2.4301
	BBBB 98	MET	14.3698	0.0738	28.6658
	BBBB 99	GLU	7.3281	4.9392	9.2392
15	BBBB 100	GLY	5.257	5.2577	0.0000
	BBBB 101	GLN	9.4091	0.0245	16.9168
	BBBB 102	PRO	9.6291	1.5760	20.3666
	BBBB 103	LEU	0.0129	0.0053	0.0206
00	BBBB 104	PHE	6.1594	0.0000	9.6790
20	BBBB 105	LEU	0.0613	0.0533	0.0693
	BBBB 106	ARG	2.2836	0.0000	3.5885
	BBBB 107	CYS	0.6725	1.0088	0.0000
	BBBB 108	HIS	1.1253	0.2267	1.7244
05	BBBB 109	GLY	1.2775	1.2775	0.0000
25	BBBB 110	TRP	4.4509	0.3060	6.1089
	BBBB 111	ARG	14.4604	6.9977	18.7248
	BBBB 112	ASN	13.1855	4.3879	21.9831
	BBBB 113	TRP	7.1019	3.5603	8.5186
20	BBBB 114	ASP	11.9934	2.2124	21.7745
30	BBBB 115	VAL	0.9738	0.8493	1.1398
	BBBB 116	TYR	5.9699	0.0003	8.9548
	BBBB 117	LYS	11.3675	0.6641	19.9301
	BBBB 118	VAL	0.0000	0.0000	0.0000
35	BBBB 119	ILE	4.4231	0.0000	8.8463
33	BBBB 120	TYR	0.0060	0.0000	0.0090
	BBBB 121	TYR	3.5477	0.0003	5.3215
	BBBB 122	LYS	3.9640	0.7211	6.5584
	BBBB 123	ASP	10.6309	6.1402	15.1215
40	BBBB 124	GLY	14.3673	14.3673	0.0000
40	BBBB 125	GLU	13.1648	0.4047	23.3729
	BBBB 126	ALA	14.7406	5.6401	51.1429
	BBBB 127	LEU	9.0669	6.2840	11.8498
	BBBB 128	LYS	11.7318	1.7962	19.6802
45	BBBB 129	TYR	10.3977	5.0068	13.0932
73	BBBB 130	TRP	8.0404	1.1151	10.8105
	8888 131 8888 132	TYR	12.1527	0.8656	17.7962
		GLU	12.6929	2.0269	21.2256
	BBBB 133	ASN	5.5740	5.4313	5.7167
50	8888 134 8888 135	HIS	8.2722	1.4837	12.7979
50		ASN	1.3495	0.3379	2.3611
	BBBB 136 BBBB 137	ILE	2.1772	1.2842	3.0701
		SER	10.0581	7.4531	15.2681
		ILE Tup	3.4589	0.9040	6.0137
55		THR	15.5520	2.5023	32.9516
J.J	BBBB 140 BBBB 141	ASN	6.4140	3.6881	9.1399
	BBBB 141	ALA	0.0003	0.0003	0.0000

	BBBB 142 BBBB 143 BBBB 144	THR VAL GLU	6.5774 7.8299 14.1982	0.3047 1.0449 4.2567	14.9409 16.8764 22.1514
5	BBBB 145 BBBB 146	ASP	4.3806	0.0466	8.7146
3	BBBB 146 BBBB 147	SER GLY	5.5841	4.1811	8.3902
	BBBB 148	THR	2.9485 5.5009	2.9485 0.1035	0.0000
	BBBB 149	TYR	0.2416	0.0180	12.6974 0.3534
	BBBB 150	TYR	3.8781	0.0000	5.8171
10	BBBB 151	CYS	0.0000	0.0000	0.0000
	BBBB 152	THR	3.8579	0.0000	9.0018
	BBBB 153	GLY	1.0286	1.0286	0.0000
	BBBB 154	LYS	6.0883	0.0037	10.9561
	BBBB 155	VAL	0.4604	0.0000	1.0742
15	BBBB 156	TRP	11.6843	J.2412	14.2615
	BBBB 157	GLN	14.2169	3.2783	22.9678
	BBBB 158	LEU	13.8111	0.3293	27.2930
	BBBB 159	ASP	14.3170	4.9359	23.6980
••	BBBB 160	TYR	3.5010	2.3021	4.1004
20	BBBB 161	GLU	13.3785	5.0194	20.0658
	BBBB 162	SER	1.1216	1.6824	0.0000
	BBBB 163	GLU	9.8626	0.5373	17.3229
	BBBB 164 BBBB 165	PRO	10.0802	1.5190	21.4953
25	BBBB 165 BBBB 166	LEU ASN	1.6748	0.1571	3.1924
23	BBBB 167	ILE	4.0864 0.5430	1.0418 1.0598	7.1311 0.0262
	BBBB 168	THR	9.9575	0.1056	23.0934
	BBBB 169	VAL	0.5482	0.9594	0.0000
	BBBB 170	ILE	10.7170	1.5437	19.8904
30	BBBB 171	LYS	20.1725	15.3137	24.0596
	BBBB 221	NAG	13.1802	0.0000	13.1802
	BBBB 222	NAG	20.4108	0.0000	20.4108
	BBBB 242	NAG	7.5051	0.0000	7.5051
	BBBB 243	NAG	7.8194	0.0000	7.8194
35	BBBB 244	MAN	18.6420	0.0000	18.6420
	BBBB 250	NAG	16.2628	0.0000	16.2628
	BBBB 274	NAG	21.8856	0.0000	21.8856
	BBBB 335	NAG	14.8369	0.0000	14.8369
40	BBBB 340 BBBB 366	NAG	17.4016	0.0000	17.4016
40	BBBB 366 BBBB 367	NAG NAG	14.6038	0.0000	14.6038
	DDDD 4	LYS	21.0874 22.1244	0.0000 10.4757	21.0874 31.4434
	DDDD 5	PRO	1.1536		•
	DDDD 6	LYS	17.0471	1.5927 1.3682	0.5680 29.5902
45	DDDD 7	VAL	1.6664	2.8596	0.0755
	DDDD 8	SER	8.3148	1.8918	21.1607
	DDDD 9	LEU	4.3290	5.2653	3.3927
	DDDD 10	ASN	12.0081	0.9613	23.0549
	DDDD 11	PRO	8.1330	0.4813	18.3353
50	DDDD 12	PRO	10.2920	2.3028	20.9442
	DDDD 13	TRP	1.5549	0.0701	2.1488
	DDDD 14	ASN	3.1974	0.3117	6.0832
	DDDD 15	ARG	1.7368	0.0000	2.7293
	DDDD 16	ILE	0.9559	0.0003	1.9114
55	DDDD 17	PHE	0.3209	0.0000	0.5043
	DDDD 18	LYS	10.9142	3.4868	16.8562

	DDDD 19	GLY	5.8859	5.8859	0.0000
	DDDD 20	GLU	3.5184	0.0001	6.3330
	DDDD 21	ASN	5.3913	4.1153	6.6672
	DDDD 22	VAL	0.2777	0.4369	0.0655
5	DDDD 23	THR	5.8162	0.1076	13.4277
	DDDD 24	LEU	0.4623	0.0006	0.9240
	DDDD 25	THR	5.1763	0.0000	12.0779
	DDDD 26	CYS	0.2817	0.3216	0.2020
	DDDD 27	ASN	8.2286	1.5680	14.8891
10	DDDD 28	GLY	7.4834	7.4834	0.0000
	DDDD 29	ASN	17.4431	8.5265	26.3597
	DDDD 30	ASN	14.3278	10.0224	18.6333
	DDDD 31	PHE	18.8219	8.9687	24.4524
	DDDD 32	PHE	7.0915	6.7608	7.2806
15	DDDD 33	GLU	17.4529	5.1261	27.3143
	DDDD 34	VAL	10.0069	3.7179	18.3922
	DDDD 35	SER	14.6436	2.2454	39.4399
	DDDD 36	SER	7.1471	1.9242	
	DDDD 37	THR	0.7333	1.2833	17.5931
20	DDDD 38	LYS	8.8058		0.0000
20	DDDD 39	TRP	0.0167	0.3191	15.5951
	DDDD 40	PHE		0.0569	0.0007
	DDDD 41	HIS	3.0699	0.0000	4.8241
	DDDD 41	ASN	3.3244	0.1639	5.4315
25	DDDD 42 DDDD 43	GLY	6.2564	7.1984	5.3143
23	DDDD 43		8.8245	8.8245	0.0000
	DDDD 45	SER	12.8423	3.1760	32.1749
	DDDD 45	LEU	14.8050	7.3234	22.2866
		SER	6.2461	4.5119	9.7144
30	DDDD 47	GLU	19.8403	7.8973	29.3948
30	DDDD 48	GLU	5.7613	2.1656	8.6379
	DDDD 49	THR	10.9341	0.0000	25.5128
	DDDD 50	ASN	3.7321	1.0782	6.3860
	DDDD 51	SER	1.1905	0.0000	3.5714
25	DDDD 52	SER	2.7666	0.0003	8.2993
35	DDDD 53	LEU	2.7642	0.0050	5.5234
	DDDD 54	ASN	7.1762	4.1170	10.2353
	DDDD 55	ILE	1.9872	1.4615	2.5130
	DDDD 56	VAL	11.4848	1.8199	24.3713
40	DDDD 57	ASN	9.2650	1.2272	17.3029
40	DDDD 58	ALA	0.3308	0.4134	0.0000
	DDDD 59	LYS	13.7555	0.1261	24.6591
	DDDD 60	PHE	4.2948	0.3462	6.5511
	DDDD 61	GLU	9.1485	0.1440	16.3520
4.00	DDDD 62	ASP	4.0350	0.0620	8.0080
45	DDDD 63	SER	0.1959	0.0000	0.5877
	DDDD 64	GLY	0.0065	0.0065	0.0000
	DDDD 65	GLU	7.8394	0.0396	14.0791
	DDDD 66	TYR	1.0148	0.0000	1.5222
	DDDD 67	LYS	3.3208	0.0000	5.9774
50	DDDD 68	CYS	0.0002	0.0000	0.0005
	DDDD 69	GLN	3.9726	0.0000	7.1507
	DDDD 70	HIS	2.6810	0.2742	4.2855
	DDDD 71	GLN	16.6353	6.3493	24.8641
	DDDD 72	GLN	18.9785	6.9612	28.5924
55	DDDD 73	VAL	5.8822	1.9838	11.0801
	DDDD 74	ASN	7.4325	0.9456	13.9195
				•	

	DDDD 75	GLU	9.6342	4.3175	13.8875
	DDDD 76	SER	0.6597	0.9801	0.0188
	DDDD 77	GLU	15.8994	1.2593	27.6115
	DDDD 78	PRO	8.2500	4.9080	12.7060
5	DDDD 79	VAL	6.5718	1.5859	13.2197
	DDDD 80	TYR	7.3618	1.8414	10.1220
	DDDD 81	LEU	0.3727	0.0000	0.7455
	DDDD 82	GLU	5.7273	0.0000	10.3091
	DDDD 83	VAL	1.6083	2.8146	0.0000
10	DDDD 84	PHE	2.9246	0.6110	4.2466
	DDDD 85	SER	11.0966	6.0084	21.2730
	DDDD 86	ASP	6.2089	2.2133	10.2046
	DDDD 87	TRP	6.4962	0.2557	8.9923
	DDDD 88	LEU	0.0479	0.0958	0.0000
15	DDDD 89	LEU	0.1157	0.0000	0.2313
	DDDD 90	LEU	0.0002	0.0000	0.0004
	DDDD 91	GLN	0.2632	0.0000	0.4737
	DDDD 92	ALA	0.0436	0.0427	0.0472
	DDDD 93	SER	4.5089	2.9688	7.5891
20	DDDD 94	ALA	8.3925	1.3517	36.5557
	DDDD 95	GLU	7.1932	1.4693	11.7724
	DDDD 96	VAL	13.5421	4.7333	25.2870
	DDDD 97	VAL	1.5725	0.9243	2.4367
	DDDD 98	MET	14.2776	0.0883	28.4668
25	DDDD 99	GLU	7.6854	4.8779	9.9313
	DDDD 100	GLY	4.9621	4.9621	0.0000
	DDDD 101	GLN	9.7282	0.0319	17.4852
	DDDD 102	PRO	9.4269	1.5462	19.9345
	DDDD 103	LEU	0.0306	0.0330	0.0282
30	DDDD 104	PHE	6.2490	0.0000	9.8199
	DDDD 105	LEU	0.0962	0.0653	0.1272
	DDDD 106	ARG	2.2407	0.0007	3.5207
	DDDD 107	CYS	0.6463	0.9694	0.0000
	DDDD 108	HIS	1.1583	0.2394	1.7709
35	DDDD 109	GLY	1.3558	1.3558	0.0000
	DDDD 110	TRP	4.6167	0.3206	6.3351
	DDDD 111	ARG	13.1658	6.9018	16.7453
	DDDD 112	ASN	12.9428	4.3861	21.4995
	DDDD 113	TRP	6.0476	2.8196	7.3388
40	DDDD 114	ASP	11.3414	1.8363	20.8466
	DDDD 115	VAL	0.8809	0.7036	1.1174
	DDDD 116	TYR	5.3412	0.0000	
	DDDD 117	LYS	8.0269	0.7095	8.0118 13.8809
	DDDD 118	VAL	0.0001	0.0000	0.0002
45	DDDD 119	ILE	1.6342	0.0000	3.2684
	DDDD 120	TYR	0.0131	0.0000	0.0197
	DDDD 121	TYR	2.9992	0.0083	4.4947
	DDDD 122	LYS	4.0023	0.8041	6.5609
	DDDD 123	ASP	10.7259	6.1708	
50	DDDD 124	GLY	14.3365	14.3365	15.2810 0.0000
-	DDDD 125	GLU	7.3185	0.3720	
	DDDD 126	ALA	2.1423	1.1064	12.8756
	DDDD 127	LEU	5.9 <b>56</b> 9	1.10 <del>04</del> 1.4445	6.2860
	DDDD 128	LYS	11.1254	0.27 <b>8</b> 5	10.4694
55	DDDD 129	TYR	5.7025	4.2384	19.8028
	DDDD 130	TRP	6.8913		6.4346
	2220 100	1135	0.0313	1.0864	9.2132

	DDDD 131	TYR	4.0982	0.8881	5.7033
	DDDD . 132	GLU	11.0810	2.0497	18.3061
	DDDD 133	ASN	5.7438	5.5427	5.9449
	DDDD 134	HIS	8.0681	1.4827	12.4583
5	DDDD 135	ASN	1.3522	0.3616	2.3429
	DDDD 136	ILE	2.1277	1.2709	2.9846
	DDDD 137	SER	10.0928	7.5360	15.2065
	DDDD 138	ILE	3.4325	0.8858	5.9792
	DDDD 139	THR	15.7856	2.5286	33.4616
10	DDDD 140	ASN	6.3849	3.6475	9.1223
	DDDD 141	ALA	0.0000	0.0000	0.0000
	DDDD 142	THR	7.3411	0.2496	16.7963
	DDDD 143	VAL	7.7635	1.1808	16.5403
. ~	DDDD 144	GLU	13.9706	4.2430	21.7527
15	DDDD 145	ASP	4.2654	0.0465	8.4843
	DDDD 146	SER	5.4380	3.9844	8.3451
	DDDD 147	GLY	2.9908	2.9908	0.0000
	DDDD 148	THR	5.6821	0.0926	13.1348
20	DDDD 149	TYR	0.2615	0.0000	0.3922
20	DDDD 150	TYR	3.8602	0.0001	5.7903
	DDDD 151	CYS	0.0000	0.0000	0.0000
	DDDD 152	THR	3.8063	0.0000	8.8814
	DDDD 153	GLY	1.1071	1.1071	0.0000
25	DDDD 154	LYS	5.9720	0.0003	10.7494
25	DDDD 155	VAL	0.4744	0.0002	1.1066
	DDDD 156	TRP	3.1754	2.8159	3.3193
	DDDD 157 DDDD 158	GLN	10.0034	3.2877	15.3759
		LEU	14.1226	0.2738	27.9715
30	DDDD 159 DDDD 160	ASP	7.9805	2.3321	13.6289
50		TYR	3.5343	2.4074	4.0978
	DDDD 161 DDDD 162	GLU SER	12.6759	4.6202	19.1204
	DDDD 162	GLU	1.1111	1.6667	0.0000
	DDDD 163	PRO	9.9628	0.6047	17.4493
35	DDDD 165	LEU	10.2553	1.5732	21.8314
33	DDDD 166	ASN	1.6609 4.3037	0.1704	3.1515
	DDDD 167	ILE	4.3037 0.5355	1.0892	7.5182
	DDDD 168	THR	9.9863	1.0632 0.0926	0.0079
	DDDD 169	VAI	0.5843	0.9875	23.1779
40	DDDD 170	ILE	10.6158	1.4450	0.0466
	DDDD 171	LYS	20.3127	15.3369	19.7865 24.2933
	DDDD 221	NAG	13.3953	0.0000	13.3953
	DDDD 222	NAG	19.9723	0.0000	19.9723
	DDDD 242	NAG	9.9403	0.0000	9.9493
45	DDDD 243	NAG	9.3637	0.0000	9.3637
	DDDD 244	MAN	18.7429	0.0000	18.7429
	DDDD 250	NAG	16.0945	0.0000	16.0945
	<b>DDDD 274</b>	NAG	21.9996	0.0000	21.9996
	DDDD 335	NAG	15.1906	0.0000	15.1906
50	DDDD 340	NAG	17.8940	0.0000	17.8940
	DDDD 366	NAG	14.6791	0.0000	14.6791
	<b>DDDD 367</b>	NAG	20.8557	0.0000	20.8557
	EEEE 4	LYS	22.5960	10.2165	32.4995
	EEEE 5	PRO	1.1597	1.6130	0.5553
55	EEEE 6	LYS	16.8781	1.3580	29.2941
	EEEE 7	VAL	1.6131	2.7766	0.0619
				•	

	EEEE 8	SER	8.2297	1.9067	20.8757
	EEEE 9	LEU	4.4542	5.4841	3.4242
	EEEE 10	ASN	11.9578	0.9345	22.9812
_	EEEE 11	PRO	8.0892	0.4787	18.2367
5	EEEE 12	PRO	10.2667	2.2261	20.9875
	EEEE 13	TRP	1.5846	0.0803	2.1863
	EEEE 14	ASN	3.3863	0.3258	6.4468
	EEEE 15	ARG	1.7357	0.0000	2.7275
	EEEE 16	ILE	0.9829	0.0000	1.9657
10	EEEE 17	PHE	0.3246	0.0002	0.5100
	EEEE 18	LYS	10.8388	3.5327	16.6837
	EEEE 19	GLY	5.3803	5.3803	0.0000
	EEEE 20	GLU	3.5458	0.0335	6.3557
	EEEE 21	ASN	5.3181	4.0487	6.5875
15	EEEE 22	VAL	0.2825	0.4415	0.0706
	EEEE 23	THR	5.3581	0.0670	12.4128
	EEEE 24	LEU	0.4756	0.0000	0.9513
	EEEE 25	THR	5.2190	0.0000	12.1778
•	EEEE 26	CYS	0.3475	0.4090	0.2246
20	EEEE 27	ASN	8.6206	1.5643	15.6770
	EEEE 28	GLY	7.3744	7.3744	0.0000
	EEEE 29	ASN	16.8741	8.5078	25.2404
	EEEE 30	ASN	14.4860	9.6381	19.3339
0.5	EEEE 31	PHE	18.9288	9.2491	24.4601
25	EEEE 32	PHE	7.2780	<b>6.7628</b>	7.5723
	EEEE 33	GLU	17.3776	4.9213	27.3427
	EEEE 34	VAL	9.8146	3.7193	17.9417
	EEEE 35	SER	14.4525	2.2438	38.8698
20	EEEE 36	SER	7.1292	1.8233	17.7410
30	EEEE 37	THR	0.7268	1.2719	0.0000
	EEEE 38	LYS	8.8146	0.3416	15.5930
	EEEE 39	TRP	0.0112	0.0389	0.0002
	EEEE 40	PHE	3.0771	0.0000	4.8354
35	EEEE 41	HIS	3.3339	0.3893	5.2969
33	EEEE 42	ASN	6.3403	7.2548	5.4 <b>25</b> 9
	EEEE 43	GLY	8.8849	8.8849	0.0000
	EEEE 44	SER	12.3851	3.1501	30.8551
	EEEE 45	LEU	14.5997	6.7706	22.4287
40	EEEE 46 EEEE 47	SER	6.2344	4.5208	9.6615
40		GLU	19.8124	8.1501	29.1422
	EEEE 48	GLU	5.5829	2.2603	8.2411
	EEEE 49	THR	11.1823	0.0000	26.0920
	EEEE 50	ASN	3.7514	1.0379	6.4648
45	EEEE 51	SER	1.1828	0.0001	3.5482
40	EEEE 52	SER	2.6847	0.0000	8.0542
	EEEE 53	LEU	2.8988	0.0160	5.7815
	EEEE 54	ASN	7.0295	3.8406	10.2183
	EEEE 55	ILE	1.9774	1.5267	2.4282
50	EEEE 56	VAL	11.4385	1.7455	24.3625
30	EEEE 57	ASN	8.9737	1.1309	16.8164
	EEEE 58	ALA	0.3534	0.4418	0.0000
	EEEE 59	LYS	14.0513	0.0995	25.2128
	EEEE 60	PHE	3.9435	0.0489	6.1690
55	EEEE 61	GLU	9.2441	0.1331	16.5329
JJ	EEEE 62	ASP	4.0153	0.0793	7.9514
	EEEE 63	SER	. 0.1893	0.0000	0.5678

	EEEE 64	GLY	0.0000	0.0000	0.0000
	EEEE 65	GLU	2.9838	0.0460	5.3340
	EEEE 66	TYR	1.0048	0.0006	1.5069
	EEEE 67	LYS	3.2772	0.0001	5.8989
5	EEEE 68	CYS	0.0000	0.0000	0.0000
	EEEE 69	GLN	3.9654	0.0000	7.1378
	EEEE 70	HIS	2.6414	0.2451	4.2389
	EEEE 71	GLN	9.7531	6.2755	12.5353
10	EEEE 72	GLN	15.3796	6.7847	22.2555
10	EEEE 73	VAL	6.0006	2.3479	10.8709
	EEEE 74	ASN	7.6007	0.9858	14.2156
	EEEE 75	GLU	9.6042	4.4474	13.7297
	EEEE 76	SER	0.6746	1.0066	0.0106
15	EEEE 77	GLU	12.7067	1.2232	21.8935
15	EEEE 78	PRO	2.3956	1.5978	3.4593
	EEEE 79	VAL	6.0444	0.7862	13.0553
	EEEE 80 EEEE 81	TYR	4.1212	1.3782	5.4928
		LEU	0.4531	0.0000	0.9061
20	EEEE 82 EEEE 83	GLU VAL	5.5155	0.0000	9.9279
20	EEEE 84	PHE	1.5309	2.6784	0.0008
	EEEE 85		2.8834	0.6355	4.1679
	EEEE 86	SER ASP	11.0911	6.1575	20.9584
	EEEE 87	TRP	6.4143	2.5687	10.2598
25	EEEE 88	LEU	9.2857	0.2426	12.9030
~~	EEEE 89	LEU	0.0519 0.1205	0.1037	0.0000
	EEEE 90	LEU	0.1205	0.0000	0.2410
	EEEE 91	GLN	0.2686	0.0000 0.0000	0.0000
	EEEE 92	ALA	0.0943	0.0991	0.4835
30	EEEE 93	SER	4.2341	2.9403	0.0752 6.8217
	EEEE 94	ALA	8.4724	1.4590	36.5259
	EEEE 95	GLU	4.3753	1.4778	6.6933
	EEEE 96	VAL	4.5984	4.5523	4.6599
	EEEE 97	VAL	1.5521	0.9731	2.3241
35	EEEE 98	MET	14.3494	0.0687	28.6301
	EEEE 99	GLU	7.4147	5.0436	9.3116
	EEEE 100	GLY	5.3477	5.3477	0.0000
	EEEE 101	GLN	9.6429	0.0120	17.3476
	EEEE 102	PRO	9.4892	1.6653	19.9211
40	EEEE 103	LEU	0.0234	0.0192	0.0275
	EEEE 104	PHE	6.1 <b>968</b>	0.0000	9.7379
	EEEE 105	LEU	0.0865	0.0657	0.1072
	EEEE 106	ARG	2.2169	0.0000	3.4838
	EEEE 107	CYS	0.6436	0.9654	0.0000
45	EEEE 108	HIS	1.1724	0.2409	1.7935
	EEEE 109	GLY	1.2996	1.2996	0.0000
	EEEE 110	TRP	4.6388	0.3429	6.3572
	EEEE 111	ARG	14.4865	6.9035	18.8197
50	EEEE 112	ASN	13.2482	4.3960	22.1003
50	EEEE 113	TRP	7.0238	3.3035	8.5119
	EEEE 114	ASP	11.8883	1.9586	21.8181
	EEEE 115	VAL	0.8842	0.7257	1.0956
	EEEE 116	TYR	6.0204	0.0000	9.0306
55	EEEE 117	LYS	11.3486	0.7247	19.8476
JJ	EEEE 118 EEEE 119	VAL.	0.0000	0.0000	0.0000
	EEEE 119	ILE	4.3850	. 0.0000	8.7700

---

	EEEE 120	TYR	0.0002	0.0005	0.0000
	EEEE 121	TYR	3.8442	0.0044	5.7642
	EEEE 122	LYS	4.0492	0.9747	6.5088
	EEEE 123	ASP	10.6363	6.3573	14.9153
5	EEEE 124	GLY	14.2853	14.2853	0.0000
	EEEE 125	GLU	13.3618	0.4051	23.7272
	EEEE 126	ALA	14.6809	5.6541	50.7878
	EEEE 127	LEU	9.2613	6.4361	12.0866
	EEEE 128	LYS	11.7127	1.6189	19.7878
10	EEEE 129	TYR	10.5042	5.1382	13.1872
	EEEE 130	TRP	8.3076	1.0723	11.2017
	EEEE 131	TYR	12.1072	0.8991	17.7113
	EEEE 132	GLU	12.7199	2.0028	21.2936
	EEEE 133	ASN	5.6925	5.5621	5.8228
15	FFEE 134	HIS	8.1921	1.5201	12.6401
	EEEE 135	ASN	1.3201	0.2942	2.3461
	EEEE 136	ILE	2.2145	1.3058	3.1231
	EEEE 137	SER	10.0571	7.3406	15.4902
	EEEE 138	ILE	3.4381	0.9086	5.9677
20	EEEE 139	THR	15.7625	2.5279	33.4087
	EEEE 140	ASN	6.4209	3.6811	9.1607
	EEEE 141	ALA	0.0000	0.0000	0.0000
	EEEE 142	THR	7.2538	0.3369	16.4763
	EEEE 143	VAL	5.2826	1.1302	10.8192
25	EEEE 144	GLU	14.2599	4.2746	22.2482
	EEEE 145	ASP	4.3200	0.0534	8.5866
	EEEE 146	SER	5.5098	4.0762	8.3771
	EEEE 147	GLY	2.9433	2.9433	0.0000
•	EEEE 148	THR	5.7039	0.0995	13.1764
30	EEEE 149	TYR	0.2552	0.0130	0.3763
	EEEE 150	TYR	3.8275	0.0000	5.7413
	EEEE 151	CYS	0.0000	0.0000	0.0000
	EEEE 152	THR	3.7660	0.0000	8.7874
0.5	EEEE 153	GLY	1.1095	1.1095	0.0000
35	EEEE 154	LYS	6.0705	0.0037	10.9239
	EEEE 155	VAL	0.4853	0.0000	1.1323
	EEEE 156	TRP	11.8745	5.3 <b>33</b> 7	14.4908
	EEEE 157	GLN	14.3320	3.3004	23.1573
40	EEEE 158	LEU	13.6525	0.2539	27.0512
40	EEEE 159	ASP	14.3336	5.0741	23.5931
	EEEE 160	TYR	3.5095	2.3905	4.0689
	EEEE 161	GLU	13.4677	5.2742	20.0225
	EEEE 162	SER	1.1284	1.6927	0.0000
45	EEEE 163	GLU	9.6823	0.5318	17.0027
45	EEEE 164	PRO	10.3139	1.5274	22.0292
	EEEE 165	LEU	1.6379	0.1485	3.1273
	EEEE 166	ASN	3.3639	0.7774	5.9503
	EEEE 167	ILE	0.5534	1.0911	0.0157
50	EEEE 168	THR	3.6331	0.0674	8.3873
50	EEEE 169	VAL.	0.0817	0.1078	0.0468
	EEEE 170	ILE	2.1648	0.0777	4.2519
	EEEE 171	LYS	14.9019	13.4622	16.0537
	EEEE 221	NAG	13.0723	0.0000	13.0723
55	EEEE 222	NAG	20.3453	0.0000	20.3453
55	EEEE 242	NAG	8.8452	0.0000	8.8452
	EEEE 243	NAG	7.6625	0.0000	7.6625

-422-

	EEEE 244	MAN	18.6073	0.0000	18.6073
	EEEE 250	NAG	16.1217	0.0000	16.1217
	EEEE 274	NAG	22.0349	0.0000	22.0349
	EEEE 335	NAG	15.0552	0.0000	15.0552
5	EEEE 340	NAG	17.7238	0.0000	17.7238
	EEEE 366	NAG	12.1825	0.0000	12.1825
	EEEE 367	NAG	19.5820	0.0000	19 5820

Table 11. PhFcεRIα₁₋₁₇₆, Form M2, residue exposure

>>>> coordinate set= md6c1.pdb

	segid	resid	resname	access	access-main	access-side
5	AAAA	1	VAL	23.3378	10.2131	40.8375
	AAAA	2	PRO	11.8969	4.7510	21.4247
	AAAA	3	GLN	4.0040	0.6188	6.7120
	AAAA	4	LYS	10.6487	3.0641	16.7164
	AAAA	5	PRO	0.2700	0.1467	0.4343
10	AAAA	6	LYS	14.5164	0.1128	26.0393
	AAAA	7	VAL	2.0175	3.5306	0.0002
	AAAA	8	SER	8.4156	1.5950	22.0570
	AAAA	9	LEU	3.4044	3.6981	3.1106
	AAAA	10	ASN	11.5698	0.5893	22.5503
15	AAAA	11	PRO	8.5175	0.1465	19.6787
	AAAA	12	PRO	9.1363	1.5259	19.2835
	AAAA	13	TRP	2.0981	0.0033	2.9360
	AAAA	14	ASN	2.7536	0.0000	5.5073
	AAAA	15	ARG	0.7887	0.0000	1.2394
20	AAAA	16	ILE	0.5825	0.0000	1.1649
	AAAA	17	PHE	0.1853	0.0000	0.2912
	AAAA	18	LYS	9.6106	1.2098	16.3312
	AAAA	19	GLY	4.3200	4.3200	0.0000
	AAAA	20	GLU	2.6272	0.0000	4.7290
25	AAAA	21	ASN	4.7245	2.9284	6.5206
	AAAA	22	VAL	0.4741	0.6955	0.1788
	AAAA	23	THR	4.7669	0.0001	11.1226
	AAAA	24	LEU	0.0001	0.0000	0.0002
	AAAA	25	THR	5.8774	0.0006	13.7131
30	AAAA	26	CYS	1.2474	1.8711	0.0000
	AAAA	27	ASN	9.8972	1.4492	18.3453
	AAAA	28	GLY	11.8125	11.8125	0.0000
	AAAA	29	ASN	10.4976	5.7985	15.1967
	AAAA	30	ASN	17.1596	4.7289	29.5903
35	AAAA	31	PHE	14.9024	9.0487	18.2474
	AAAA	32	PHE	6.9262	1.1011	10.2548
	AAAA	33	GLU	19.3638	7.9005	28.5344
	AAAA	34	VAL	10.5040	9.2873	12.1262
	AAAA	35	SER	20.0797	11.1239	37.9912
40	AAAA	36	SER	10.3115	2.5541	25.8262
	AAAA	37	THR	0.3123	0.1509	0.5275
	AAAA	38	LYS	9.1055	0.0303	16.3656
	AAAA	39	TRP	0.0125	0.0004	0.0173
	AAAA	40	PHE	3.3329	0.0507	5.2085
45	AAAA	41	HIS	3.3604	0.4369	5.3093
	AAAA	42	ASN	5.7196	5.9748	5.4644
	AAAA	43	GLY	11.0441	11.0441	0.0000
	AAAA	44	SER	12.3468	1.6054	33.8295
	AAAA	45	LEU	12.4194	6.6727	18.1661
50	AAAA	46	SER	6.2970	3.5164	11.8583
	AAAA	47	GLU	19.2754	6.3506	29.6153
	AAAA	48	GLU	5.5497	2.2183	8.2149
	AAAA	49	THR	10.8597	1.3240	23.5740

	AAAA	50	ASN	12.0836	1.0849	23.0822
	AAAA	.51	SER	8.5667	0.8380	24.0243
	AAAA	52	SER	6.5795	0.5607	18.6170
	AAAA	53	LEU	2.0088	0.0000	4.0175
5	AAAA	54	ASN	10.4631	4.8106	16.1155
	AAAA	55	ILE	1.5373	1.3922	1.6825
	AAAA	56	VAL	9.8664	4.5674	16.9318
	AAAA	57	ASN	8.3728	1.0485	15.6970
	AAAA	58	ALA	0.1673	0.2091	0.0000
10	AAAA	59	LYS	12.7698	0.0135	22.9748
	AAAA	60	PHE	2.9685	0.0000	4.6647
	AÀAA	61	GLU	10.1438	0.3798	17.9550
	AAAA	62	ASP	3.8187	0.0000	7.6375
	AAAA	63	SER	0.0423	0.0002	0.1265
15	AAAA	64	GLY	0.7550	0.7550	0.0000
	AAAA	65	GLU	4.0298	0.0243	7.2343
	AAAA	66	TYR	0.5144	0.0000	0.7716
	AAAA	67	LYS	4.6070	0.0021	8.2910
	AAAA	68	CYS	0.0643	0.0965	0.0000
20	AAAA	69	GLN	4.3129	0.5930	7.2889
	AAAA	70	HIS	2.2107	1.4131	2.7425
	AAAA	71	GLN	15.8607	4.7123	24.7794
	AAAA	72	GLN	10.1949	4.9757	14.3702
25	AAAA	73	VAL	4.5886	3.4088	6.1618
25	AAAA	74	ASN	7.2228	1.6554	12.7903
	AAAA	<b>75</b>	GLU	11.1970	3.1686	17.6196
	AAAA AAAA	76	SER	0.7529	1.1293	0.0000
	AAAA	77 78	GLU PRO	5.6624	0.5155	9.7799
30	AAAA	70 79	VAL	9.4668	4.0586	16.6776
50	AAAA	80	TYR	4.2206	0.7903	8.7943
	AAAA	81	LEU	10.8696	1.6448	15.4820
	AAAA	82	GLU	0.3 <b>29</b> 5 6.5599	0.6590	0.0000
	AAAA	83	VAL	1.2313	0.0000 2.1548	11.8078
35	AAAA	84	PHE	2.6783	1.0628	0.0000 3.6015
	AAAA	85	SER .	10.4042	7.2453	16.7222
	AAAA	86	ASP	6.7155	3.1365	10.7222
	AAAA	87	TRP	7.9670	0.0000	11.1538
	AAAA	88	LEU	0.2303	0.4605	0.0000
40	AAAA	89	LEU	0.1824	0.0005	0.3643
	AAAA	90	LEU	0.0000	0.0000	0.0000
	AAAA	91	GLN	0.1542	0.0000	0.2776
	AAAA	92	ALA	0.0000	0.0000	0.0000
	AAAA	93	SER	6.4731	4.6474	10.1245
45	AAAA	94	ALA	6.9800	1.7371	27.9520
	AAAA	95	GLU	6.3625	0.8834	10.7457
	AAAA	96	VAL	12.7032	5.5496	22.2413
	AAAA	97	VAL	1.4127	0.9895	1.9769
	AAAA	98	MET	8.3663	0.9908	15.7417
50	AAAA	99	GLU	6.0466	3.8025	7.8419
	AAAA	100	GLY	1.3823	1.3823	0.0000
	AAAA	101	GLN	9.3401	0.0000	16.8122
	AAAA	102	PRO	11.5211	1.3350	25.1025
	AAAA	103	LEU	0.2239	0.2968	0.1510
55	AAAA	104	PHE	5.5960	0.0000	8.7937
	AAAA	105	LEU	0.2800	. 0.0000	0.5599

WO 00/26246

-425-

	AAAA	106	ARG	5.6019	0.0000	8.8030
	AAAA	107	CYS	1.9041	2.6369	0.4387
	AAAA	108	HIS	1.2459	0.8447	1.5133
	AAAA	109	GLY	0.2958	0.2958	0.0000
5	AAAA	110	TRP	3.6776	0.2682	5.0414
	AAAA	111	ARG	13.9748	6.0118	18.5251
	AAAA	112	ASN	13.0426	5.9312	20.1540
	AAAA	113	TRP	8.4374	2.2626	10.9073
	AAAA	114	ASP	10.8862	0.8382	20.9341
10	AAAA	115	VAL	3.6736	4.0353	3.1913
	AAAA	116	TYR	10.8526	0.9359	15.8110
	AAAA	117	LYS	12.5729	4.0303	19.4070
	AAAA	118	VAL	1.5367	1.4181	1.6949
	AAAA	119	ILE	3.8886	0.4794	7.2979
15	AAAA	120	TYR	0.1235	0.0400	0.1653
	AAAA	121	TYR	3.2159	0.0000	4.8238
	AAAA	122	LYS	4.1348	0.5235	7.0239
	AAAA	123	ASP	9.0341	4.7242	13.3440
20	AAAA	124	GLY	12.8886	12.8 <b>88</b> 6	0.0000
20	AAAA	125	GLU	13.5568	0.5821	23.9366
	AAAA	126	ALA	5.4 <del>44</del> 8	3.6508	12.6207
	AAAA	127	LEU	4.4392	1.2148	7.6637
	AAAA	128	LYS	6.6847	0.4089	11.7054
05	AAAA	129	TYR	17.7661	6.5522	23.3730
25	AAAA	130	TRP	4.6781	0.2956	6.4311
	AAAA	131	TYR	5.9070	2.3743	7.6733
	AAAA	132	GLU	14.4146	6.3584	20.8595
	AAAA	133	ASN	9.2636	0.7631	17.7642
30	AAAA	134	HIS	14.3143	1.4912	22.8630
30	AAAA	135	ASN	6.6861	0.2683	13.1040
	AAAA AAAA	136	ILE	0.1409	0.0100	0.2719
	AAAA	137 138	SER	9.4451	3.2255	21.8842
	AAAA	139	ILE THR	2.6491	0.8829	4.4154
35	AAAA	140	ASN	12.8859 6.4 <del>4</del> 32	1.4417	28.1448
55	AAAA	141	ALA		3.5706	9.3157
	AAAA	142	THR	1.3406 7.2752	1.6757	0.0000
	AAAA	143	VAL		0.0020	16.9727
	AAAA	144	GLU	11.7608 14.7507	1.2461	25.7803
40	AAAA	145	ASP	3.5866	2.5626	24.5012
••	AAAA	146	SER	4.2659	0.0546 2.0709	7.1186
	AAAA	147	GLY	4.2659 2.4870		8.6561
	AAAA	148	THR	3.9797	2.4870 0.0000	0.0000
	AAAA	149	TYR	0.3266	0.0000	9.2860
45	AAAA	150	TYR	3.1527	0.0005	0.4899
	AAAA	151	CYS	0.0003	0.0005	4.7289 0.0000
	AAAA	152	THR	4.1824	0.6979	8.8283
	AAAA	153	GLY	0.7331	0.7331	
	AAAA	154	LYS	7.5163	0.0133	0.0000
50	AAAA	155	VAL	0.2906	0.0000	13.5188
	AAAA	156	TRP	11.8912	1.7474	0.6781 15.9487
	AAAA	157	GLN	14.6241	5.4565	21.9582
	AAAA	158	LEU	13.5291	0.9340	
	AAAA	159	ASP	14.3755	5.4004	26.1242 23.3507
55	AAAA	160	TYR	3.1668	2.6149	3.4428
	AAAA	161	GLU	10.8144	4.2630	16.0556
	· •			, , , ,		10.0000

	AAAA	162	SER	0.5614	0.8334	0.0172
	AAAA	163	GLU	10.6063	0.2900	18.8593
	AAAA	164	PRO	10.9414	3.3661	21.0417
	AAAA	165	LEU	1.9287	0.7267	3.1308
5	AAAA	166	ASN	5.8142	3.0970	8.5314
	AAAA	167	ILE	0.2918	0.5835	0.0000
	AAAA	168	THR	9.3327	0.0000	21.7764
	AAAA	169	VAL	0.2835	0.4961	0.0000
	AAAA	170	ILE	10.1702	0.5659	19.7745
10	AAAA	171	LYS	14.8660	3.9580	23.5925
	AAAA	172	ALA	10.1636	3.7167	35.9516
	AAAA	173	PRO	16.8141	8.4692	27.9405
	AAAA	174	ARG	24.7335	21.3158	26.6865
15	AAAA	221	NAG	10.3017	0.0000	10.3017
15	AAAA	222	NAG	20.4990	0.0000	20.4990
	AAAA	242	NAG	10.4998	0.0000	10.4998
	AAAA	243	NAG	9.1915	0.0000	9,1915
	AAAA	244	MAN	17.0951	0.0000	17.0951
20	AAAA	274	NAG	8.2536	0.0000	8.2536
20	AAAA	275	FCA	13.5116	0.0000	13.5116
	AAAA	276	NAG	18.0492	0.0000	18.0492
	AAAA AAAA	340	NAG	18.2117	0.0000	18.2117
	BBBB	366	NAG	20.2201	0.0000	20.2201
25	BBBB	1 2	VAL PRO	23.2202	13.0224	36.8172
23	BBBB	3	GLN	12.9287	6.5376	21.4502
	BBBB	4	LYS	7.8969	1.1767	13.2731
	BBBB	5	PRO	10.9639	2.4069	17.8095
	8888	6	LYS	0.1485 13.6900	0.1774	0.1101
30	BBBB	7	VAL	2.0335	0.3136	24.3911
	BBBB	8	SER	8.6515	3.5586 1.6168	0.0000
	BBBB	9	LEU	3.3843	3.6519	22.7209
	BBBB	10	ASN	11.2166	0.5892	3.1168 21.8441
	BBBB	11	PRO	6.4967	0.0774	15.0558
35	BBBB	12	PRO	5.5258	1.4792	10.9213
	BBBB	13	TRP	0.5399	0.0000	0.7559
	888B	14	ASN	2.8551	0.0000	5.7102
	BBBB	15	ARG	0.8228	0.0000	1.2930
	BBBB	16	ILE	0.7004	0.0000	1.4007
40	BBBB	17	PHE	0.2062	0.0000	0.3240
	BBBB	18	LYS	10.1266	2.4178	16.2937
	BBBB	19	GLY	5.1193	5.1193	0.0000
	BBBB	20	GLU	3.6592	0.0000	6.5866
	8888	21	ASN	4.9980	2.8696	7.1265
45	BBBB	22	∨AL	0.3086	0.5358	0.0056
	BBBB	23	THR	4.8914	0.0060	11.4053
	8888	24	LEU	0.0000	0.0000	0.0000
	BBBB	25	THR	5.3161	0.0000	12.4043
50	BBBB	26	CYS	1.7698	1.9470	1.4152
50	BBBB	27	ASN	9.5595	2.4594	16.6596
	BBBB	28	GLY	5.1022	5.1022	0.0000
	BBBB	29	ASN	11.6239	9.1902	14.0577
	BBBB	30	ASN	11.1354	7.5265	14.7442
55	BBBB	31	PHE	12.4823	0.9411	19.0773
55	8888	32	PHE	14.9629	4.4534	20.9683
	BBBB	33	GLU	10.0579	. 1.1430	17.1898

	BBBB 34	VAL	8.1169	2.1335	16.0948
	BBBB .35	SER	17.2091	9.6972	32.2329
	BBBB 36	SER	5.6660	1.8677	13.2627
_	BBBB 37	THR	0.9190	0.7693	1.1187
5	BBBB 38	LYS	10.5493	0.0585	18.9418
	BBBB 39	TRP	0.0160	0.0000	0.0224
	BBBB 40	PHE	3.2085	0.1128	4.9774
	BBBB 41	HIS	3.2674	0.7993	4.9129
	BBBB 42	ASN	6.9206	7.0588	6.7824
10	BBBB 43	GLY	10.5521	10.5521	0.0000
	BBBB 44	SER	12.5873	1.8007	34.1606
	BBBB 45	LEU	12.5684	7.0671	18.0697
	BBBB 46	SER	5.8736	2.9025	11.8159
	BBBB 47	GLU	18.2898	4.6076	29.2356
15	BBBB 48	GLU	6.4732	2.2413	9.8587
	BBBB 49	THR	12.4950	1.2186	27.5302
	BBBB 50	ASN	10.6353	1.9696	19.3010
	BBBB 51	SER	2.7922	0.0131	8.3506
20	BBBB 52	SER	5.4540	0.4267	15.5085
20	BBBB 53	LEU	2.2138	0.0004	4.4271
	BBBB 54	ASN	10.5005	4.6511	16.3499
	BBBB 55	ILE	1.3385	1.1102	1.5667
	BBBB 56	VAL	11.5067	3.9707	21.5548
25	BBBB 57	ASN	8.7141	1.1097	16.3 <b>185</b>
25	BBBB 58	ALA	0.1840	0.2300	0.0000
	BBBB 59	LYS	13.0236	0.0000	23.4424
	BBBB 60	PHE	2.3308	0.0000	3.6627
	BBBB 61	GLU	9.4233	0.1906	16.8095
30	BBBB 62	ASP	3.8339	0.0000	7.6678
30	BBBB 63 BBBB 64	SER	0.1605	0.0000	0.4815
	BBBB 64 BBBB 65	GLY	1.6421	1.6421	0.0000
	BBBB 66	GLU TYR	3.9224	0.0377	7.0302
	BBBB 67	LYS	0.5105	0.0000	0.7658
35	BBBB 68	CYS	3.9749	0.0002	7.1547
JJ	BBBB 69	GLN	0.0929	· 0.1393	0.0000
	BBBB 70	HIS	5.4367	0.1443	9.6707
	BBBB 71	GLN	4.9806 14.5333	0.9868	7.6431
	BBBB 72	GLN	18.4063	5.4826	21.7740
40	BBBB 73	VAL	2.6548	11.6333	23.8247
10	BBBB 74	ASN	12.0029	3.2121	1.9118
	0000		8.4921	2.0287	21.9770
	BBBB 75	GLU SER	0.7254	2.6890	13.1345
	BBBB 77	GLU	7.7802	1.0881	0.0000
45	BBBB 78	PRO	9.3860	0.6132	13.5138
	BBBB 79	VAL	4.0363	3.7419	16.9114
	BBBB 80	TYR	11.1782	0.8626 1.6916	8.2679
	BBBB 81	LEU	0.2983	0.5965	15.9215
	BBBB 82	GLU	7.4968	0.0000	0.0000
50	BBBB 83	VAL	1.2876	2.2532	13.4942
	BBBB 84	PHE	2.7723	1.0285	
	BBBB 85	SER	10.1939	7.3007	3.7688 15.9804
	BBBB 86	ASP	6.5079	7.3007 3.0391	
	BBBB 87	TRP	6.1336	0.0000	9.9768
55	BBBB 88	LEU	0.2766	0.5478	8.5870 0.0054
	BBBB 89	LEU	0.2222	0.0049	0.4394
	<del></del>		·	0.0073	0.4084

	BBBB	90	LEU	0.0152	0.0302	0.0001
	BBBB	91	GLN	0.1468	0.0000	0.2642
	BBBB		ALA	0.0005	0.0006	0.0000
_	BBBB		SER	5.6156	4.5602	7.7265
5	BBBB		ALA	6.8297	1.8546	26.7302
	BBBB		GLU	6.8738	0.8762	11.6719
	BBBB		VAL	12.2316	5.3212	21.4456
	BBBB		VAL	1.4488	1.1013	1.9123
10	BBBB	98	MET	11.2447	0.4365	22.0530
10	BBBB		GLU	6.9392	5.4744	8.1110
	BBBB		GLY	2.1371	2.1371	0.0000
	BBBB		GLN	10.3142	0.0031	18.5631
	BBBB	102	PRO	10.9007	1.3692	23.6094
15	BBBB	103	LEU	0.1806	0.2907	0.0705
13	BBBB	104	PHE	0.9676	0.0002	1.5204
	BBBB	105	LEU	0.2088	0.0016	0.4161
	BBBB BBBB	106 107	ARG	3.6986	0.0002	5.8119
	BBBB	108	CYS HIS	0.0292	0.0438	0.0000
20	BBBB	109	GLY	1.4195	0.6184	1.9535
20	BBBB	110	TRP	0.5887	0.5887	0.0000
	BBBB	111	ARG	0.8590 12.1336	0.0000	5.4025
	8888	112	ASN		6.9873	15.0744
	BBBB	113	TRP	13.9325 3.3478	3.3709 2.2053	24.4942
25	BBBB	114	ASP	7.6950	2.2053 3.0188	3.8048 - 12.3711
	BBBB	115	VAL	0.1840	0.2489	0.0975
	BBBB	116	TYR	4.9222	0.0000	7.3832
	BBBB	117	LYS	10.4451	0.8887	18.0902
	BBBB	118	VAL	0.0000	0.0000	0.0000
30	BBBB	119	ILE	4.6639	0.0004	9.3274
	BBBB	120	TYR	0.0002	0.0000	0.0003
	BBBB	121	TYR	3.8872	0.0000	5.8308
	BBBB	122	LYS	4.3212	0.6213	7.2812
	BBBB	123	ASP	9.3317	5.1768	13.4866
35	BBBB	124	GLY	14.0149	14.0149	0.0000
	BBBB	125	GLU	14.1323	1.6253	24.1378
	BBBB	126	ALA	12.2018	6.3993	35.4121
	BBBB	127	LEU	9.7819	5.9893	13.5746
40	BBBB	128	LYS	10.6006	2.2370	17.2915
40	BBBB	129	TYR	9.1175	4.6166	11.3680
	BBBB	130	TRP	11.8627	0.8908	16.2515
	BBBB	131	TYR	9.3270	0.4323	13.7744
	BBBB	132	GLU	10.1438	0.0000	18.2588
45	BBBB	133	ASN	4.9699	1.6521	8.2877
43	BBBB	134	HIS	2.1605	0.1201	3.5207
	BBBB	135	ASN	3.4385	4.8744	2.0027
	8888 8888	136	ILE	0.1878	0.2608	0.1149
	8888	137 138	SER	10.4452	5.0394	21.2570
50	BBBB	139	ILE	4.4124	0.8988	7.9260
50	8888	140	THR	13.3105	0.5909	30.2701
	8888	141	ASN ALA	6.8155	3.1228	10.5082
	BBBB	142	THR	1.3398	1.6747	0.0000
	BBBB	143	VAL	7.5421	0.0097	17.5852
55	BBBB	144	GLU	11.6452 14.1708	1.2806	25.4646
	BBBB	145	ASP	3.4895	1.1173	24.6136
		. 10	7.01	0.4030	. 0.0584	6.9206

	BBBB	146	SER	4.2945	1.9825	8.9184
	BBBB	. 147	GLY	4.3457	4.3457	0.0000
	BBBB	148	THR	4.4415	0.0000	10.3634
	BBBB	149	TYR	0.0214	0.0001	0.0321
5	BBBB	150	TYR	3.1691	0.0000	4.7537
	BBBB	151	CYS	0.0000	0.0000	0.0000
	BBBB	152	THR	3.5053	0.0000	8.1791
	BBBB	153	GLY	0.6931	0.6931	0.0000
	BBBB	154	LYS	6.3103	0.0180	11.3441
10	BBBB	155	VAL	0.0365	0.0044	0.0793
	BBBB	156	TRP	3.3899	5.9121	2.3810
	BBBB	157	GLN	16.5870	5.2100	25.6886
	BBBB	158	LEU	13.1911	0.1922	26.1899
	BBBB	159	ASP	13.0965	5.2133	20.9797
15	BBBB	160	TYR	3.2939	3.1627	3.3595
	BBBB	161	GLU	10.8490	4.6790	15.7 <b>851</b>
	BBBB	162	SER	0.5960	0.7781	0.2318
	BBBB	163	GLU	10.5937	0.3366	18.7993
	BBBB	164	PRO	11.6713	3.2190	22.9411
20	8888	165	LEU	1.9716	0.7957	3.1476
	BBBB	166	ASN	5.2287	2.2398	8.2176
	BBBB	167	ILE	0.2784	0.5568	0.0000
	BBBB	168	THR	9.3922	0.0000	21.9152
	8888	169	VAL	0.2895	0.5066	0.0000
25	BBBB	170	ILE	9.7952	0.6056	18.9 <b>84</b> 8
	BBBB	171	LYS	14.9992	3.9650	23.8265
	BBBB	172	ALA	8.6682	3.2571	30.3128
	BBBB	173	PRO	17.2332	8.4 <b>40</b> 5	28.9567
•	BBBB	174	ARG	24.5074	21.0894	26.4605
30	BBBB	221	NAG	17.4850	0.0000	17.4850
	BBBB	242	NAG	10.4355	0.0000	10.4355
	BBBB	243	NAG	10.3502	0.0000	10.3502
	BBBB	244	MAN	15.8885	0.0000	15.8 <b>88</b> 5
	BBBB	335	NAG	8.8279	0.0000	8.8279
35	BBBB	336	NAG	16.5384	0.0000	16.5384
	BBBB	337	FCA	16.2107	0.0000	16.2107
	BBBB	340	NAG	13.5916	0.0000	13.5916
	BBBB	341	NAG	21.2819	0.0000	21.2819
	BBBB	366	NAG	21.9238	0.0000	21.9238

Table 12. PhFceRI $\alpha_{1-172}$ , Form H1, residue exposure

>>>> coordinate set= c703f.pdb

	segid		فيانون	qe accessible	area
	<u>sidechain</u>	<u>resid</u>	resname	residue	mainchain
5	1	VAL	22.5900	15.0637	32.6251
	2	PRO	11.2478	3.9295	21.0055
	3	GLN	15.8860	3.9559	25.4300
	4	LYS	7.8658	4.1508	10.8378
	5	PRO	0.7859	0.7412	0.8456
10	6	LYS	15.0743	0.2689	26.9185
	7	VAL	2.5158	4.4026	0.0000
	8	SER	8.7041	1.7476	22.6170
	9	LEU	3.4804	4.2930	2.6678
	10	ASN	13.3748	1.0394	25.7103
15	11	PRO	6.4372	0.6223	14.1904
	12	PRO	9.9906	1.9726	20.6812
	13	TRP	1.6444	0.0463	2.2837
	14	ASN	2.4971	0.0178	4.9764
	15	ARG	1.2172	0.0001	1.9127
20	16	ILE	0.3947	0.0000	0.7895
20	17	PHE	0.1203	0.0000	0.1890
	18	LYS	9.6134	1.5661	16.0512
	19	GLY	6.4465	6.4465	0.0000
	20	GLU	2.9946	0.0000	5.3903
25	21	ASN	4.7501	2.8416	6.6586
23	22	VAL	0.3670	0.6423	0.0000
	23	THR	5.0060	0.1082	11.5364
	24	LEU	0.2483	0.0000	0.4966
	25	THR	4.0121	0.0000	9.3616
30	26	CYS	0.1821	0.1881	0.1702
30	27	ASN	6.6425	2.1781	11.1069
	28	GLY	5.3679	5.3679	0.0000
	29	ASN	17.4099	6.2098	28.6100
	30	ASN	10.2762	3.8525	16.6998
35	31	PHE	8.0955	2.8330	11.1027
33	32	PHE	13.6377	6.1749	17.9021
	33	GLU	14.0698	3.4930	22.5313
	34	VAL	17.4046	4.8614	34.1288
	35	SER	19.6721	12.8131	33.3901
40	36	SER	11.0819	4.5899	24.0659
40	37	THR	0.8916	0.1902	1.8268
	38	LYS	8.3803	0.0158	15.0719
	39	TRP	0.0119	0.0000	0.0167
	40	PHE	3.9461	0.0636	6.1646
45	41	HIS	3.7169	0.6731	5.7461
73	42	ASN	6.6160	8.2911	4.9408
	43	GLY	11.9937	11.9937	0.0000
	43 44	SER	11.8169	1.4187	32.6133
	4 <del>4</del> 45	LEU	12.1877	6.2251	18.1503
50	45 46	SER	4.5272	3.1407	7.3002
<b>J</b> U	47	GLU		5.5809	
	47 48	GLU	18.3989		28.6533
	40	GLU	1.6700	0.3535	2.7232

	49	THR	6.8437	0.4232	15.4044
	50	ASN	6.1820	1.4496	10.9145
	51	SER	8.4271	1.0315	23.2182
	52	SER	6.0403	0.9347	16.2516
5	53	LEU	1.9666	0.0000	3.9331
	54	ASN	10.6560	4.7155	16.5965
	55	ILE	1.5407	1.0849	1.9965
	56	VAL	8.4966	4.2813	14.1170
	57	ASN	8.0710	0.2994	15.8427
10	58	ALA	0.4475	0.5594	0.0000
	59	LYS	12.6628	0.0000	22.7931
	60	PHE	2.0470	0.0207	3.2050
	61	GLU	9.1096	0.1120	16.3076
٠,٠	62	ASP	3.9382	0.0000	7.8765
15	63	SER	0.1178	0.0000	0.3535
	64 65	GLY	0.5477	0.5477	0.0000
	65	GLU	3.5925	0.1947	6.3107
•	66	TYR	0.3061	0000.0	0.4592
20	67 68	LYS	4.9263	0.0000	8.8674
20	68 60	CYS	0.0002	0.0002	0.0000
	69 70	GLN	3.1065	0.1191	5.4965
	70 71	HIS GLN	4.3287	0.5494	6.8482
	71 72	GLN	14.4511 16.7254	4.6243	22.3126
25	72 73	VAL	4.6849	5.5984	25.6271
23	74	ASN	3.7390	0.0239 2.2152	10.8997
	<b>75</b>	GLU	9.8220	1.6123	5.2628 16.3897
	76	SER	0.9279	1.3599	0.0638
	77	GLU	10.2035	0.8100	17.7182
30	78	PRO	6.8952	4.7323	9.7791
	79	VAL	4.4704	0.8249	9.3311
	80	TYR	10.8485	1.3619	15.5919
	81	LEU	0.8740	1.0895	0.6586
	82	GLU	6.2336	0.0000	11.2205
35	83	VAL	1.6724	2.9266	0.0000
	84	PHE	3.0301	0.8580	4.2712
	85	SER	10.9935	6.5698	19.8409
	86	ASP	6.6012	2.2575	10.9449
	87	TRP	9.0703	0.2059	12.6161
40	88	LEU	0.4451	0.8570	0.0331
	89	LEU	0.5432	0.0676	1.0187
	90	LEU	0.0913	0.1298	0.0527
	91	GLN	0.0763	0.0000	0.1373
4 50	92	ALA	0.0388	0.0480	0.0022
45	93	SER	4.5675	4.1995	5.3034
	94	ALA	7.1276	1.0786	31.3237
	95 96	GLU	6.8795	1.2919	11.3495
	96 07	VAL	13.0247	4.2238	24.7593
50	97 98	VAL	1.0770	0.5985	1.7150
50	99	MET	16.7988	0.4914	33.1061
	100	GLU GLY	7.5393	3.3688	10.8758
	100	GLY	3.1157	3.1157	0.0000
	102	PRO	10.1587	0.2304	18.1014
55	103	LEU	8.7856 0.0405	1.4883	18.5154
	104	PHE	5.7390	0.0000 0.0000	0.0810
			J.1 J3U	0.0000	9.0184

	105	LEU	0.0000	0.0000	0.0000
	106	ARG	4.9770	0.0000	7.8210
	107	CYS	2.8329	3.8594	0.7800
	108	HIS	1.0226	0.3429	1.4757
5	109	GLY	0.7524	0.7524	0.0000
J	110	TRP	4.3881	0.0000	6.1433
	111	ARG	13.1221	5.0820	17.7164
	112	ASN	12.3893	5.7597	19.0188
	113	TRP	6.4754	2.8590	7.9219
10	114	ASP	11.2956	2.1441	20.4471
10	115	VAL	2.0499	2.1826	1.8731
	116	TYR	11.1258	1.0112	16.1831
	117	LYS	16.7863	4.7622	26.4055
	117	VAL	8.1424	6.0958	10.8711
15	119	ILE	6.8012	0.9964	12.6060
15	120	TYR	2.8442	0.9061	3.8133
	121	TYR	3.5867	0.0012	5.3794
	122	LYS	5.1214	0.6012	8.7376
	123	ASP	7.4941	4.6376	10.3507
20	124	GLY	12.2128	12.2128	0.0000
20	125	GLU	15.1128	1.2362	26.2141
	126	ALA	11.6923	3.6139	44.0058
	127	LEU	4.6471	5.4019	3.8923
	128	LYS	18.8922	6.6649	28.6740
25	129	TYR	17.4834	7.0989	22.6757
25	130	TRP	2.4961	4.3542	1.7528
	131	TYR	12.7233	5.2485	16.4608
	132	GLU	13.6661	0.7556	23.9944
	133	ASN	9.3922	6.3761	12.4084
30	134	HIS	15.2795	8.2917	19.9381
20	135	ASN	11.1940	2.7459	19.6420
	136	ILE	5.4540	0.6821	10.2259
	137	SER	0.6915	0.0000	2.0744
	138	ILE	6.3883	1.6352	11.1413
35	139	THR	4.7987	2.2363	8.2152
22	140	ASN	5.2615	2.7779	7.7451
	141	ALA	0.9545	1.1931	0.0000
	142	THR	6.9219	0.6069	15.3420
	143	VAL	9.5663	1.8575	19.8448
40	144	GLU	14.4371	3.2860	23.3579
40	145	ASP	2.2220	0.0056	4.4384
	146	SER	5.2393	2.1712	11.3756
	147	GLY	3.0536	3.0536	0.0000
	148	THR	2.8393	0.0000	6.6250
45	149	TYR	0.0489	0.0000	0.0734
15	150	TYR	3.3061	0.0181	4.9500
	151	CYS	0.0000	0.0000	0.0000
	152	THR	3.7148	0.0000	8.6679
	153	GLY	0.9412	0.9412	0.0000
50	154	LYS	8.4275	0.1238	15.0704
50	155	VAL	0.3174	0.0138	0.7223
	156	TRP	14.1884	7.2900	16.9477
	157	GLN	15.4584	4.5161	24.2122
	158	LEU	11.5234	0.7276	22.3193
55	159	ASP	15.3714	7.3517	23.3910
	160	TYR	4.5849	1.8192	5.9678

PCT/US99/26203

**-433**-

			•		
	161	GLU	12.0528	4.8779	17.7927
	162	SER	0.9680	1.3220	0.2601
	163	GLU	10.9265	0.9944	18.8722
	164	PRO	11.4182	2.7638	22.9575
5	165	LEU	1.8797	0.4866	3.2727
_	166	ASN	5.1428	2.5621	7.7235
	167	ILE	0.3717	0.7433	0.0000
	168	THR	9.9155	0.0000	23.1363
	169	VAL	0.2713	0.4747	0.0000
10	170	ILE	12.6290	1.6535	23.6046
	171	LYS	18.1223	11.6928	23.2660
	221	NAG	10.3807	0.0000	10.3807
	222	NAG	20.2927	0.0000	20.2927
	242	NAG	10.3379	0.0000	10.3379
15	243	NAG	10.0051	0.0000	10.0051
	244	MAN	17.1981	0.0000	17.1981
	250	NAG	15.4600	0.0000	15.4600
	274	NAG	20.0516	0.0000	20.0516
	340	NAG	16.0149	0.0000	16.0149
20	341	NAG	20.8951	0.0000	20.8951
	366	NAG	14.4348	0.0000	14.4348
	367	NAG	20.6913	0.0000	20.6913

Table 13. Crystallographic data and model refinement

one and	10.000	5m/QF		50 m <b>1</b> 2
res.	3.2	3.2	3.1	3.8
wavel(A)	1.0039	1.0047	0.914	0.92
comp/(last shell)	93.2(95.4)	99.3(100)	97.0(83.3)	85.7(80.2)
av. red. (last shell)	8.0(7.1)	4.1(4.2)	7.3(2.2)	2.0(1.6)
Rmerge (last shell)	10.3(51.6)	9.7(43.6)	11.2(76.6)	6.3(60.9)
l/sigi (last shell)	11.8(5.3)	9.2(3.0)	7.9(1.1)	7.5(1.1)
#refl(free)	4030(412)	11640(620)	23318(1180)	14239(740)
Rfactor/Rfree	28.8/31.3	25.4/28.3	29.1/32.9	27.8/30.4
# atoms	1537	3120	7660	7660
# waters	0	0	0	0
RMSD bonds	0.0084	0.0096	0.0100	0.0086
RMSD angles	1.53	1.60	1.50	1.40
Ave. B	97.1	69.4	137.6	191.1

15

10

5

Table 14. Root mean square deviations for alpha carbon positions

nodela	EMSE v. orgi(Anga)	#OA	sephoens It II
Н1	0.855	155	4-27/28-31/36-70/73-129/137-171
H1 30 loop	3.667	6	27-31, 36
H1 130 loop	4.176	9	129-137
			<b>*</b>
M2 copy A	0.880	157	4-27/36-130/134-171
M2A 30 loop	5.212	6	27-31, 36
M2A 130 loop	3.818	5	130-134
М2 сору В	0.766	155	4-27/36-127/133-171
M2B 30 loop	4.258	6	27-31, 36
M2B 130 loop	6.938	7	127-133 .
		, -	
T1 copy C	0.839	155	4-28/36-71/73-127/133-171
T1C 30 loop	6.372	5	28-31, 36
T1C 130 loop	7.449	7	127-133
		,	·
T2 copy C	0.867	155	4-28/36-71/73-127/133-171
T1C 30 loop	6.319	5	28-31, 36
T1C 130 loop	7.476	7	127-133

While various embodiments of the present invention have been described in detail, it is apparent that modifications and adaptations of those embodiments will occur to those skilled in the art. It is to be expressly understood, however, that such modifications and adaptations are within the scope of the present invention, as set forth in the following claims.

## What is claimed is:

- 1. A three-dimensional model selected from the group consisting of: (a) a three-dimensional model of an extracellular domain of a human high affinity Fc epsilon receptor alpha chain (FceRla) protein, wherein said model substantially represents the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7, and Table 8; and (b) a three-dimensional model comprising a modification of said model of (a), wherein said modification represents a protein that binds to a Fc domain of an antibody.
- 2. A method to produce a three-dimensional model of an extracellular domain of a human FceRIa protein, said method comprising representing amino acids of said protein at substantially the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8.
- 3. A method to produce a three-dimensional model of an antibody receptor protein other than a human FceRIa protein represented by the three-dimensional model substantially representing the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8, said method comprising homology modeling.
  - 4. An isolated crystal of an extracellular domain of a FceRIa protein.
- 5. A method to produce an isolated crystal of an extracellular domain of a FceRIa protein, said method comprising vapor diffusion.
- 6. An isolated FceRIa protein selected from the group consisting of: (a) a protein consisting of SEQ ID NO:2; (b) a protein consisting of SEQ ID NO:4 except that the isoleucine at position 170 is replaced with a cysteine; and (c) a protein that is structurally homologous to a protein of (a) or (b), wherein said protein of (c) binds to a Fc domain of an antibody.
- 7. A method to identify a compound that inhibits the binding between an IgE antibody and a FceRIa protein, said method comprising using a three-dimensional model of an extracellular domain of a human high affinity FceRIa protein to identify said compound, wherein said model substantially represents the atomic coordinates

specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8.

- 8. A mutein that binds to a Fc domain of an antibody, wherein said mutein has an improved function compared to a protein comprising an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4, wherein said improved function is selected from the group consisting of increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, wherein said mutein is produced by a method comprising:
  - (a) analyzing a three-dimensional model substantially representing the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8 to identify at least one amino acid of the protein represented by said model which if replaced by a specified amino acid would effect said improved function of said protein; and
  - (b) replacing said identified amino acid(s) to produce said mutein having said improved function.
- 9. A mutein having an improved function compared to an unmodified FceRIa protein, wherein said improved function is selected from the group consisting of increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, wherein the amino acid sequence of said mutein differs in at least one position from the amino acid sequence of said unmodified protein, said position being in a region selected from the group consisting of a crystal contact cluster, a tryptophan-containing hydrophobic ridge, a FG loop in D2, a D1D2 interface, a cleft between D1 and D2, a domain 1, a domain 2, a hydrophobic core, a A'B loop of D1, a EF loop of D1, a BC loop of D2, a C strand of D2, a CC' loop of D2, a C'E loop of D2, a strand of D2, the amino terminal five residues of said protein, and the carboxyl terminal five residues of said protein.
- 10. A method to improve a function of a FceRIa protein, said improved function being selected from the group consisting of increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, said method comprising:

- (a) analyzing a three-dimensional model of an extracellular domain of a human high affinity FcεRIα protein substantially representing the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8 to identify at least one amino acid of said protein which if replaced by a specified amino acid improves at least one of said functions of said protein; and
- (b) replacing said identified amino acid(s) to produce a mutein having at least one of said improved functions.
- 11. An isolated FceRIa protein selected from the group consisting of: a crystal contact cluster involved in IgE binding; a tryptophan-containing hydrophobic ridge; a FG loop in D2; a D1D2 interface; a cleft between D1 and D2; a domain 1; a domain 2; a hydrophobic core; a A'B loop of D1; a EF loop of D1; a BC loop of D2; a C strand of D2; a CC' loop of D2; a C'E loop of D2; and a strand of D2.
- 12. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model is represented by a method selected from the group consisting of listing the coordinates of all atoms comprising said model, providing a physical three-dimensional model, imaging said model on a computer screen, providing a picture of said model, and deriving a set of coordinates based of a picture of said model.
- 13. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model identifies the solvent accessibility of amino acid residues of said protein listed in a table selected from the group consisting of Table 2, Table 9, Table 10, Table 11 and Table 12.
- 14. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model represents a protein that binds to a Fc domain of an IgE antibody with an affinity that is at lesst equivalent to the affinity of the extracellular domain of human FcεRIα for an IgE antibody selected from the group consisting of a human IgE antibody, a canine IgF antibody, a feline IgE antibody, an equine IgE antibody, a rat IgE antibody, and a murine IgE antibody.
- 15. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model represents a protein that selectively binds to a mammalian antibody selected from the group consisting of an IgE antibody and an IgG antibody.

- 16. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model represents an extracellular domain of a protein selected from the group consisting of a human FcεRIα protein, a canine FcεRIα protein, a feline FcεRIα protein, an equine FcεRIα protein, a murine FcεRIα protein, and a rat FcεRIα protein.
- 17. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model comprises a three-dimensional model of an extracellular antibody binding domain of an antibody receptor protein other than human FceRIa.
- 18. The invention of Claim 17, wherein said model is produced by incorporating all or any part of the amino acid sequence of said other antibody receptor protein into a three-dimensional model of said extracellular domain of said human FceRIa protein to produce said model of said other antibody receptor protein.
- 19. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model represents an IgE binding domain.
- 20. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model is produced by a method comprising:
  - (a) crystallizing an extracellular domain of a human FceRIa protein;
  - (b) collecting X-ray diffraction data from said crystallized protein; and
  - (c) determining said model from said data and amino acid sequence of said protein.
- 21. The invention of Claim 20, wherein said protein has an amino acid sequence selected from the group consisting of SEQ ID NO:2, SEQ ID NO:4 and SEQ ID NO:4 except that the isoleucine at position 170 is replaced with a cysteine.
- 22. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model has a three-dimensional structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 10 angstroms when superimposed on said three-dimensional model substantially represented by the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7, and Table 8.

- 23. The invention of Claim 1, wherein said modification has an amino acid sequence that shares at least about 30% amino acid sequence homology with a FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4.
- 24. The invention of Claim 1 or 3, wherein said model represents a FcεRIα protein having increased stability compared to the stability of a human FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4.
- 25. The invention of Claim 1 or 3, wherein said model represents a FcεRIα protein having increased affinity for IgE compared to the affinity of a human FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4 for IgE.
- 26. The invention of Claim 1 or 3, wherein said model represents a FcεRiα protein having altered substrate affinity compared to the affinity of a human FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4 for IgE.
- 27. The invention of Claim 1 or 3, wherein said model comprises a three-dimensional model of a FcεRIα protein having increased solubility compared to the solubility of a human FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4.
- 28. The invention of Claim 1, 2 or 3, wherein said model is used to identify an inhibitor of the selective binding between a FcεRIα protein and an IgE antibody.
- 29. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model identifies crystal contacts between a FcεRIα protein and a Fc domain of an IgE antibody.
- 30. The invention of Claim 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 or 11, wherein domain 1 and domain 2 are oriented in a manner as specified by the structural coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8.
- 31. The invention of Claim 1, 2, 3, 7, 8, or 10, wherein said model identifies amino acids in the D1D2 interface.

- 32. The invention of Claim 3, wherein said method of homology modeling comprises incorporating at least a portion of the amino acid sequence of said other antibody receptor protein into said three-dimensional model substantially representing the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8 to produce said model of said other antibody receptor protein.
- 33. The invention of Claim 1, 2, 3, 4, 5, or 6, wherein said protein has an amino acid sequence selected from the group consisting of SEQ ID NO:2, SEQ ID NO:4, and SEQ ID NO:4 except that the isoleucine at position 170 is replaced with a cysteine.
- 34. The invention of Claim 4 or 5, wherein said crystal belongs to a space group selected from the group consisting of monoclinic space group C2, hexagonal space group P6₁22, and tetragonal space group P4₃.
- 35. The invention of Claim 4 or 5, wherein said crystal is selected from the group consisting of: a monoclinic space group C2 having cell dimensions of 88.6 angstroms x 69.6 angstroms x 49.3 angstroms, alpha=gamma=90.0 degrees, beta=116.69 degrees; a monoclinic space group C2 having cell dimensions of 136.02 angstroms x 75.01 angstroms x 79.28 angstroms, alpha=gamma=90 degrees, beta=117.8 degrees; a monoclinic space group C2 having cell dimensions of 136.90 angstroms x 73.79 angstroms x 79.40 angstroms, alpha=gamma=90 degrees, beta=117.74 degrees; a tetragonal space group P43 having cell dimensions of 145.08 angstroms x 145.08 angstroms x 62.74 angstroms, alpha=beta=gamma=90 degrees; a tetragonal pace group P43 having cell dimensions of 150.50 angstroms x 150.50 angstroms x 74.18 angstroms, alpha=beta=gamma=90 degrees; a hexagonal space group P6122 having cell dimensions of 58 angstroms x 58 angstroms x 226 angstroms, alpha=beta=90 degrees, gamma=120 degrees; and a hexagonal space group P6122 having cell dimensions of 58.62 angstroms x 229.19 angstroms, alpha=beta=90 degrees, gamma=120 degrees.
- 36. The invention of Claim 4, 5, 6, or 11, wherein said protein is produced in insect cells or Chinese hamster ovary cells.

- 37. The invention of Claim 4 or 5, wherein said crystal diffracts X-rays to a resolution selected from the group consisting of about 2.4 angstroms, about 3.1 angstroms, about 3.2 angstroms, and about 3.8 angstroms.
- 38. The invention of Claim 1, 3, 4, 5, 6, 7, 9 or 11, wherein said protein represented by said modification of Claim 1, said antibody receptor protein of Claim 3, or said FcεRIα protein of Claim 4, 5, 6, 7, 9 or 11 is selected from the group consisting of a human FcεRIα protein, a feline FcεRIα protein, a canine FcεRIα protein, an equine FcεRIα protein, a murine FcεRIα protein, and a rat FcεRIα protein.
- 39. A nucleic acid molecule comprising a nucleic acid sequence that encodes a protein selected from the group consisting of said protein of Claim 6 or 11 and said mutein of Claim 8, 9, or 10.
  - 40. A recombinant molecule comprising a nucleic acid sequence of Claim 39.
  - 41. A recombinant virus comprising a nucleic acid sequence of Claim 39.
  - 42. A recombinant cell comprising a nucleic acid sequence of Claim 39.
- 43. A method to produce a protein comprising culturing a recombinant cell of Claim 42.
- 44. An inhibitory compound identified in accordance with the method of Claim 7.
- 45. A therapeutic composition comprising an inhibitory compound of Claim 44.
- 46. A method to protect an animal from allergy, said method comprising administering to said animal an inhibitory compound of Claim 44.
- 47. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with a region of said model selected from the group consisting of the IgE binding domain, the D1D2 interface, and the clett between domain 1 and domain 2.
- 48. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with a region of said model selected from the group consisting of a A'B loop of domain 1, a EF loop of domain 1, a BC loop of domain 2, a C strand of domain 2, a CC' loop of domain 2, a C'E loop of domain 2, a F strand of domain 2, a FG loop of domain 2, and a tryptophan-containing hydrophobic ridge.

- 49. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with a region of said model in which N-linked glycosylation sites are absent.
- 50. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with an amino acid selected from the group consisting of: (a) a residue having a position in SEQ ID NO:2 or SEQ ID NO:4 selected from the group consisting of position 87, 115, 117, 118, 120-123, 128, 129, 131, 149, 153, 155 and 159; and (b) a surface residue within about 10 angstroms of any of said residues of (a).
- 51. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with an amino acid selected from the group consisting of: (a) a residue having a position in SEQ ID NO:2 or SEQ ID NO:4 selected from the group consisting of position 87, 117, 121, 123, 128, and 159; and (b) a surface residue within about 10 angstroms of any of said residues of (a).
  - 52. The invention of Claim 7, wherein said method comprises:
  - (a) generating said model, or a model of an IgE binding domain thereof, on a computer screen;
    - (b) generating the spacial structure of a compound to be tested; and
  - (c) testing to determine if said compound interacts with said IgE binding domain, wherein such an interaction indicates that said compound is capable of inhibiting said binding of an IgE antibody to a FceRIa protein.
- 53. The invention of Claim 52, wherein said step (a) includes the step of identifying one or more amino acid(s) in the IgE binding domain of said model that interact directly with the Fc domain of an IgE antibody when said Fc domain binds to said IgE binding domain.
- 54. The invention of Claim 53, wherein said compound interacts directly with one or more of said amino acid(s).
  - 55. A diagnostic reagent comprising a mutein of Claim 8, 9 or 10.
  - 56. A therapeutic composition comprising a mutein of Claim 8, 9 or 10.
- 57. A method to use a mutein of Claim 8, 9 or 10, wherein said method is selected from the group consisting of: (a) a method to protect an animal from allergy, said method comprising administering a therapeutic composition comprising said mutein

to said animal; (b) a method to detect allergy, or susceptibility thereto, in an animal, said method comprising using said mutein to detect said allergy; and (c) a method to enhance the performance of an IgE binding assay, said method comprising incorporating into said assay said mutein.

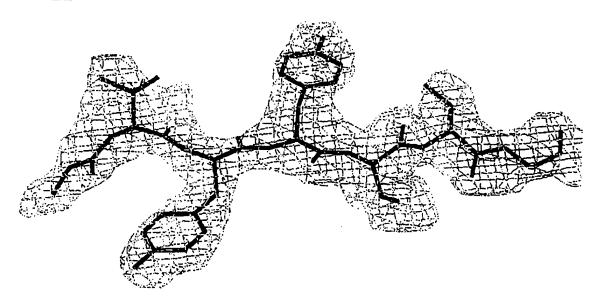
- 58. The invention of Claim 8 or 10, wherein said step of replacing does not substantially disrupt the three-dimensional structure of said protein.
- 59. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has an increased stability compared to an unmodified antibody receptor protein.
- 60. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has an increased shelf-life compared to an unmodified antibody receptor protein.
- 61. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has a K_A for said Fc domain of at least about 3 x 10⁹ liters/mole.
- 62. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has a k₄ for said Fc domain of at least about 1 x 10⁵ liters/mole-second.
- 63. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has a  $k_d$  for said Fc domain of less than or equal to 3 x 10⁻⁵/second.
- 64. The invention of Claim 8, 9 or 10, wherein said antibody is an IgE antibody.
- 65. The invention of Claim 8, 55, 56 or 57, wherein said mutein is produced by a method comprising:
  - (a) comparing the IgE binding domain on said model with amino acid sequence of an antibody receptor protein with an improved function to identify at least one amino acid segment of said antibody receptor protein with said improved function that if incorporated into said FceRIa protein represented by said model would give said FceRIa protein said improved function; and
  - (b) incorporating said segment into said FcεRIα protein, thereby producing a mutein with said improved function.
- 66. The invention of Claim 8, 10, 55, 56 or 57, wherein said mutein is produced by a method comprising:

- (a) using said model to identify a three-dimensional arrangement of residues that can be randomized by mutagenesis to allow the construction of a library of molecules from which an improved function can be selected; and
- (b) identifying at least one member of said mutagenized library having said improved function.
- 67. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein is produced by a method comprising:
  - (a) effecting random mutagenesis of nucleic acid molecules encoding a target of a FceRIa protein as identified by analyzing a model of that protein;
  - (b) cloning said mutagenized nucleic acid molecules into a phage display library, wherein said phage display library expresses said target; and
  - (c) identifying at least one member of the library that expresses said target, said target having an improved function.
- 68. The invention of Claim 67, wherein said target comprises an IgE binding domain and wherein said improved function comprises increased affinity of said domain for an antibody.
- 69. The invention of Claim 8 or 10, wherein said step of replacing is selected from the group consisting of:
  - (a) replacing at least one amino acid in at least one non-constrained loop of domain 1 in an area proximal to the FceRI gamma chain putative binding site;
  - (b) joining an amino-terminal amino acid residue to a carboxylterminal amino acid residue of an extracellular domain of a FceRIa protein;
  - (c) replacing at least one amino acid site with an amino acid suitable for derivatization:
  - (d) replacing at least one pair of amino acids of said protein with a cysteine pair to enable the formation of a disulfide bond that stabilizes said mutein;
  - (e) removing at least a portion of the region between the B strand and C strand of domain 1;

- (f) removing at least a portion of the region between the C strand and E strand of domain 1;
- (g) replacing at least one amino acid in the IgE binding domain in order to increase the affinity between an IgE antibody and said protein;
- (h) replacing at least one amino acid of said protein with an amino acid such that said replacement decreases the entropy of unfolding of said protein;
- (i) replacing at least one amino acid of said protein selected from the group consisting of asparagines and glutami as with an amino acid that is less susceptible to deamidation than is said amino acid to be replaced;
- (j) replacing at least one aminc acid of said protein selected from the group consisting of methionines, histidines and tryptophans with an amino acid that is less susceptible to an oxidation or reduction reaction than is said amino acid to be replaced;
- (k) replacing at least one arginine of said protein with an amino acid that is less susceptible to dicarbonyl compound modification than is said amino acid to be replaced;
- (l) replacing at least one amino acid of said protein susceptible to reaction with a reducing sugar sufficient to reduce said protein function with an amino acid less susceptible to said reaction;
- (m) replacing at least one amino acid of said protein with an amino acid capable of increasing the stability of the inner core of said protein;
- (n) replacing at least one amino acid of said protein with at least one N-linked glycosylation site;
- (o) replacing at least one N-linked glycosylation site of said protein with at least one amino acid that does not comprise an N-linked glycosylation site; and
- (p) replacing at least one amino acid of said protein with an amino acid that reduces aggregation of said protein.

70. The invention of Claim 8, 9, 10, 55, 56 or 57, further comprising a substance attached to an amino acid of said mutein such that said substance does not substantially interfere with the antibody binding activity of said protein.





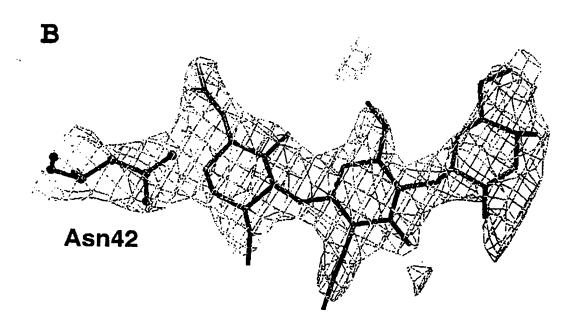
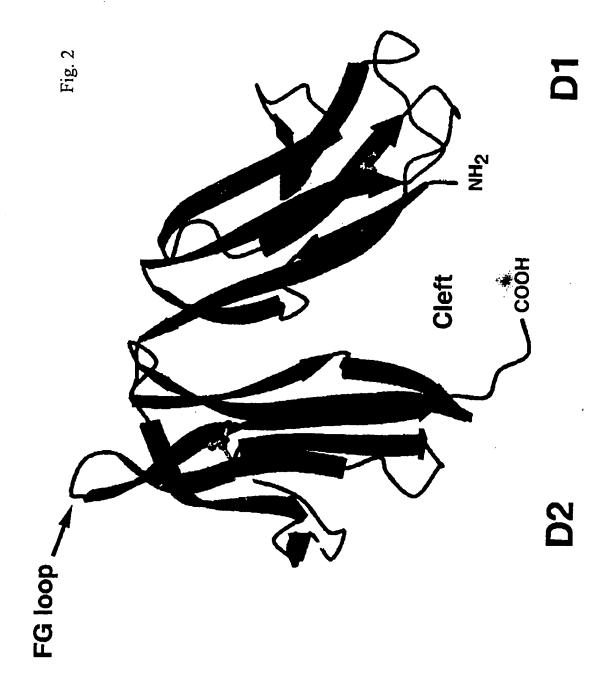
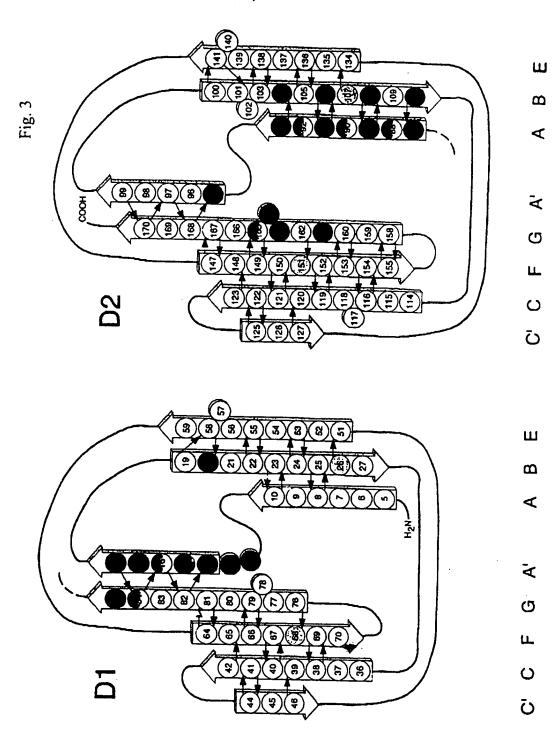


Fig. 1A, 1B





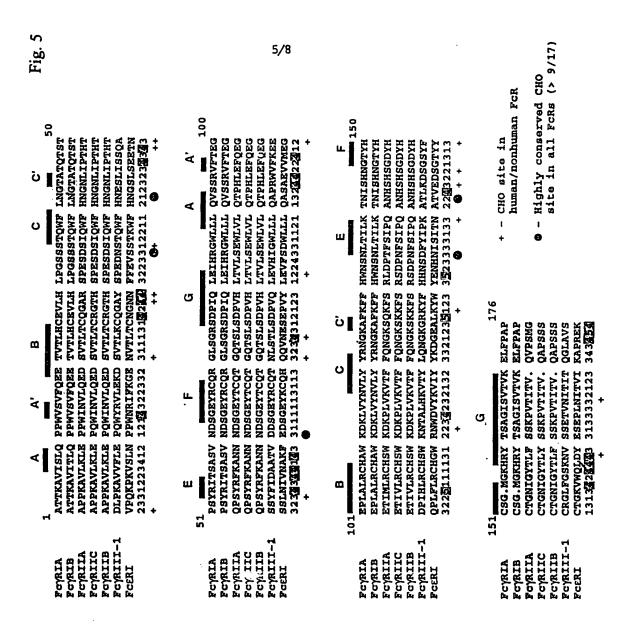
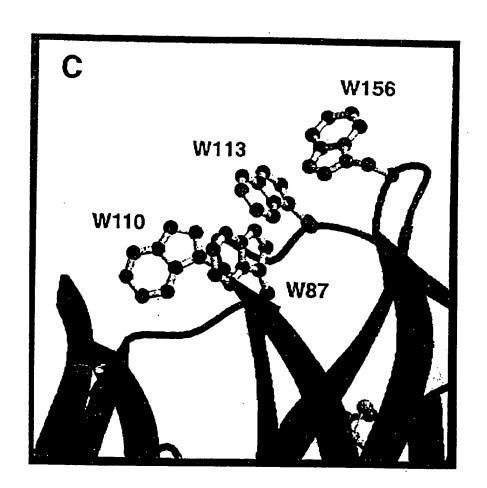


Fig. 6



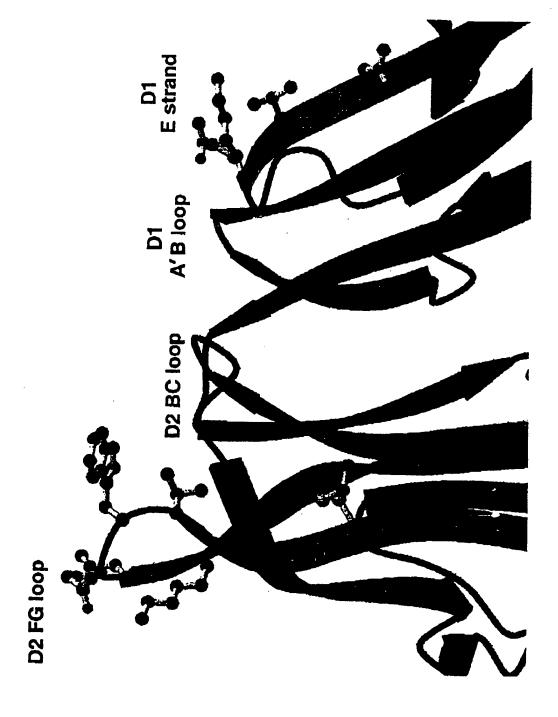
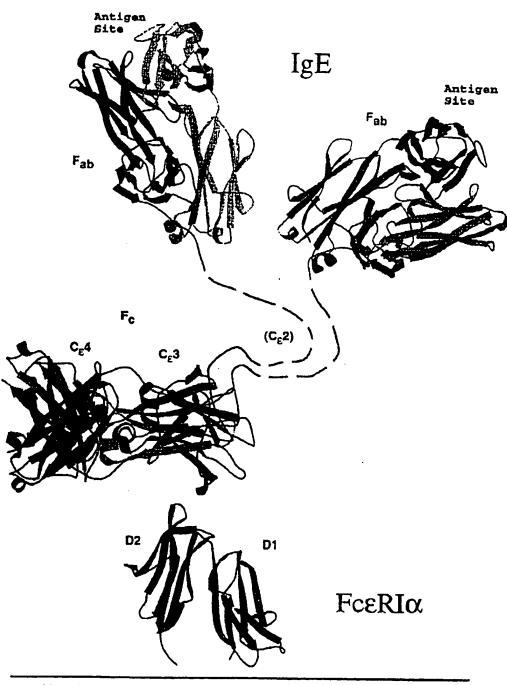


Fig. 7

Fig. 8



Mast Cell Membrane

-1-

## SEQUENCE LISTING

<pre>&lt;110&gt; Heska Corporation   Northwestern University   Jardetzky, Theodore S.   Garman, Scott Clayton   Kinet, Jean-Pierre</pre>												
:120> THREE-DIMENSIONAL MODEL OF A FC EPSILON RECEPTOR ALPHA CHAIN AND USES THEREOF												
D> HKZ-035CPPC												
10> not yet assigned 11> 1999-11-05												
<150> 60/107,219 <151> 1998-11-05												
<160> 6												
<170> PatentIn Ver. 2.0												
<210> 1 <211> 528												
<211> 526 <212> DNA												
<213> Homo sapiens												
<220> .												
<400> 1												
gtc cct cag aaa cct aag gtc tcc ttg aac cct cca tgg aat aga ata 48 Val Pro Gln Lys Pro Lys Val Ser Leu Asn Pro Pro Trp Asn Arg Ile 1 5 10 15												
ttt aaa gga gag aat gtg act ctt aca tgt aat ggg aac aat ttc ttt 96 Phe Lys Gly Glu Asn Val Thr Leu Thr Cys Asn Gly Asn Asn Phe Phe 20 25 30	ı											
gaa gtc agt tcc acc aaa tgg ttc cac aat ggc agc ctt tca gaa gag 14 Glu Val Ser Ser Thr Lys Trp Phe His Asn Gly Ser Leu Ser Glu Glu 35 40 45	4											
aca aat tca agt ttg aat att gtg aat gcc aaa ttt gaa gac agt gga 19 Thr Asn Ser Ser Leu Asn Ile Val Asn Ala Lys Phe Glu Asp Ser Gly 50 55 60	2											
gaa tac aaa tgt cag cac caa caa gtt aat gag agt gaa cct gtg tac 24 Glu Tyr Lys Cys Gln His Gln Gln Val Asn Glu Ser Glu Pro Val Tyr 65 70 75 80	0											
ctg gaa gtc ttc agt gac tgg ctg ctc ctt cag gcc tct gct gag gtg Leu Glu Val Phe Ser Asp Trp Leu Leu Gln Ala Ser Ala Glu Val 85 90 95	8											
gtg atg gag ggc cag ccc ctc ttc ctc agg tgc cat ggt tgg agg aac 33 Val Met Glu Gly Gln Pro Leu Phe Leu Arg Cys His Gly Trp Arg Asn	6											

432

480

-2-

100 105 110 tgg gat gtg tac aag gtg atc taf tat aag gat ggt gaa gct ctc aag Trp Asp Val Tyr Lys Val Ile Tyr Tyr Lys Asp Gly Glu Ala Leu Lys 120 tac tgg tat gag aac cac aac atc tcc att aca aat gcc aca gtt gaa Tyr Trp Tyr Glu Asn His Asn Ile Ser Ile Thr Asn Ala Thr Val Glu 135 gac agt gga acc tac tac tgt acg ggc aaa gtg tgg cag ctg gac tat Asp Ser Gly Thr Tyr Tyr Cys Thr Gly Lys Val Trp Gln Leu Asp Tyr 150 155 gag tot gag coc ctc aac att act gta ata aaa got cog cgt gag aag Glu Ser Glu Pro Leu Asn Ile Thr Val Ile Lys Ala Pro Arg Glu Lys <210> 2 <211> 176 <212> PRT <213> Homo sapiens <400> 2 Val Pro Gln Lys Pro Lys Val Ser Leu Asn Pro Pro Trp Asn Arg Ile Phe Lys Gly Glu Asn Val Thr Leu Thr Cys Asn Gly Asn Asn Phe Phe Glu Val Ser Ser Thr Lys Trp Phe His Asn Gly Ser Leu Ser Glu Glu Thr Asn Ser Ser Leu Asn Ile Val Asn Ala Lys Phe Glu Asp Ser Gly Glu Tyr Lys Cys Gln His Gln Gln Val Asn Glu Ser Glu Pro Val Tyr Leu Glu Val Phe Ser Asp Trp Leu Leu Leu Gln Ala Ser Ala Glu Val Val Met Glu Gly Gln Pro Leu Phe Leu Arg Cys His Gly Trp Arg Asn 100 105 Trp Asp Val Tyr Lys Val Tle Tyr Tyr Lys Asp Gly Glu Ala Leu Lys Tyr Trp Tyr Glu Asn His Asn Ile Ser Ile Thr Asn Ala Thr Val Glu 135 Asp Ser Gly Thr Tyr Tyr Cys Thr Gly Lys Val Trp Gln Leu Asp Tyr

Glu Ser Glu Pro Leu Asn Ile Thr Val Ile Lys Ala Pro Arg Glu Lys

	<21 <21	0> 3 1> 5 2> D 3> H		sapi	ens												
<220> <221> CDS <222> (1)(516)																	
	gtc	0> 3 cct Pro	cag Gln	aaa Lys	cct Pro 5	aag Lys	gtc Val	tcc Ser	ttg Leu	aac Asn 10	cct Pro	cca Pro	tgg Trp	aat Asn	aga Arg 15	ata Ile	48
	ttt Phe	aaa Lys	gga Gly	gag Glu 20	aat Asn	gtg Val	act Thr	ctt Leu	aca Thr 25	tgt Cys	aat Asn	ggg Gly	aac Asn	aat Asn 30	ttc Phe	ttt Phe	96
	gaa Glu	gtc Val	agt Ser 35	tcc Ser	acc Thr	aaa Lys	tgg Trp	ttc Phe 40	cac His	aat Asn	ggc Gly	agc Ser	ctt Leu 45	tca Ser	gaa Glu	gag Glu	144
	aca Thr	aat Asn 50	tca Ser	agt Ser	ttg Leu	aat Asn	att Ile 55	gtg Val	aat Asn	gcc Ala	aaa Lys	ttt Phe 60	gaa Glu	gac Asp	agt Ser	gga Gly	192
	gaa Glu 65	tac .Tyr	aaa Lys	tgt Cys	cag Gln	cac His 70	caa Gln	caa Gln	gtt Val	aat Asn	gag Glu 75	agt Ser	gaa Glu	cct Pro	gtg Val	tac Tyr 80	240
	ctg Leu	gaa Glu	gtc Val	ttc Phe	agt Ser 85	gac Asp	tgg Trp	ctg Leu	ctc Leu	ctt Leu 90	cag Gln	gcc Ala	tct Ser	gct Ala	gag Glu 95	gtg Val	288
	gtg Val	atg Met	gag Glu	ggc Gly 100	cag Gln	ccc Pro	ctc Leu	ttc Phe	ctc Leu 105	agg Arg	tgc Cys	cat His	ggt Gly	tgg Trp 110	agg Arg	aac Asn	336
	tgg Trp	gat Asp	gtg Val 115	tac Tyr	aag Lys	gtg Val	Ile	tat Tyr 120	tat Tyr	aag Lys	gat Asp	ggt Gly	gaa Glu 125	gct Ala	ctc Leu	aag Lys	384
	tac Tyr	tgg Trp 130	tat Tyr	gag Glu	aac Asn	cac His	aac Asn 135	atc Ile	tcc Ser	att Ile	aca Thr	aat Asn 140	gcc Ala	aca Thr	gtt Val	gaa Glu	432
	gac Asp 145	agt Ser	gga Gly	acc Thr	tac Tyr	tac Tyr 150	tgt Cys	acg Thr	ggc Gly	aaa Lys	gtg Val 155	tgg Trp	cag Gln	ctg Leu	gac Asp	tat Tyr 160	480
•	gag Glu	tct Ser	gag Glu	ccc Pro	ctc Leu 165	aac Àsn	att Ile	act Thr	gta Val	ata Ile 170	aaa Lys	gct Ala					516

<210> 4 <211> 172 <212> PRT

<213> Homo sapiens

```
<400> 4
Val Pro Gln Lys Pro Lys Val Ser Leu Asn Pro Pro Trp Asn Arg Ile
Phe Lys Gly Glu Asn Val Thr Leu Thr Cys Asn Gly Asn Asn Phe Phe
Glu Val Ser Ser Thr Lys Trp Phe His Asn Gly Ser Leu Ser Glu Glu
Thr Asn Ser Ser Leu Asn Ile Val Asn Ala Lys Phe Glu Asp Ser Gly
Glu Tyr Lys Cys Gln His Gln Gln Val Asn Glu Ser Glu Pro Val Tyr
 65
                     70
Leu Glu Val Phe Ser Asp Trp Leu Leu Gln Ala Ser Ala Glu Val
                                     90
Val Met Glu Gly Gln Pro Leu Phe Leu Arg Cys His Gly Trp Arg Asn
                                105
Trp Asp Val Tyr Lys Val Ile Tyr Tyr Lys Asp Gly Glu Ala Leu Lys
Tyr Trp Tyr Glu Asn His Asn Ile Ser Ile Thr Asn Ala Thr Val Glu
                        135
Asp Ser Gly Thr Tyr Tyr Cys Thr Gly Lys Val Trp Gln Leu Asp Tyr
Glu Ser Glu Pro Leu Asn Ile Thr Val Ile Lys Ala
<210> 5
<211> 23
<212> DNA
<213> Artificial Sequence
<223> Description of Artificial Sequence: Synthetic
      Primer
<400> 5
agctccgcgt gagaagtaat aag
                                                                  23
<210> 6
<211> 23
<212> DNA
<213> Artificial Sequence
```

<223> Description of Artificial Sequence: Synthetic

<400> 6

<220>

- 5 -

gatccttatt acttctcacg cgg

**23** .